10/784,916 8/10/05

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* * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 14:51:57 ON 10 AUG 2005

=> fil reg
COST IN U.S. DOLLARS

	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 14:52:05 ON 10 AUG 2005
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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 9 AUG 2005 HIGHEST RN 859282-03-4
DICTIONARY FILE UPDATES: 9 AUG 2005 HIGHEST RN 859282-03-4

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

Please note that search-term pricing does apply when conducting SmartSELECT searches.

****
* *
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
* *
****

Structure search iteration limits have been increased. See HELP SLIMITS for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
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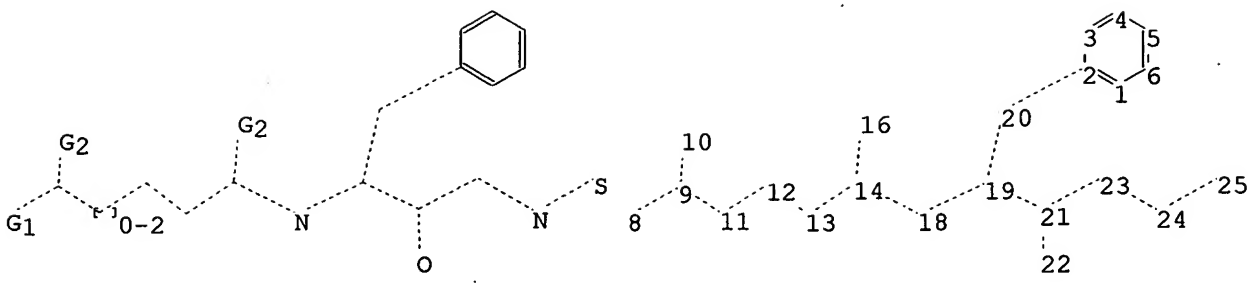

chain nodes :
8 9 10 11 12 13 14 16 18 19 20 21 22 23 24 25
ring nodes :
1 2 3 4 5 6
chain bonds :
2-20 8-9 9-10 9-11 11-12 12-13 13-14 14-16 14-18 18-19 19-20 19-21
21-22 21-23 23-24 24-25
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
2-20 8-9 9-10 9-11 11-12 12-13 13-14 14-16 14-18 18-19 19-20 19-21
21-22 21-23 23-24 24-25
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6

G1:C,O,N

G2:O,S,N

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:CLASS 9:CLASS 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 16:CLASS 18:CLASS 19:CLASS 20:CLASS
21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS

L1 STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> s L1
SAMPLE SEARCH INITIATED 14:52:42 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 110 TO ITERATE

100.0% PROCESSED 110 ITERATIONS 4 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 1571 TO 2829
PROJECTED ANSWERS: 4 TO 200

L2 4 SEA SSS SAM L1

=> s L1 full
FULL SEARCH INITIATED 14:52:46 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 2384 TO ITERATE

100.0% PROCESSED 2384 ITERATIONS 89 ANSWERS
SEARCH TIME: 00.00.01

L3 89 SEA SSS FUL L1

=> fil caplus
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 161.33 161.54

FILE 'CAPLUS' ENTERED AT 14:52:50 ON 10 AUG 2005
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FILE COVERS 1907 - 10 Aug 2005 VOL 143 ISS 7
FILE LAST UPDATED: 9 Aug 2005 (20050809/ED)

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s L3
L4 23 L3

=> d ibib abs hitstr 1-23

L4 ANSWER 1 OF 23 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2005:527407 CAPLUS
DOCUMENT NUMBER: 143:59982
TITLE: Preparation of HIV protease inhibitors, in particular imidazolidine derivatives
INVENTOR(S): Flentge, Charles A.; Chen, Hui-Ju; Degoey, David A.; Flosi, William J.; Grampovnik, David J.; Huang, Peggy P.; Kempf, Dale J.; Klein, Larry L.; Krueger, Allan C.; Madigan, Darold L.; Randolph, John T.; Sun, Minghua; Yeung, Ming C.; Zhao, Chen
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 287 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005131042	A1	20050616	US 2003-733915	20031211
WO 2005061450	A2	20050707	WO 2004-US37745	20041110

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 2003-733915 A 20031211
GI

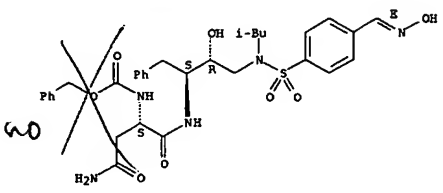
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title compds. of formula ANH(CHR)(CHR1)(CHR2)NR3S(O2)R4 (I) [wherein A = alkylcarbonyl, arylsulfonyl, 1,3-substituted 2-oxoimidazolidinyl, 2,4-dioxoimidazolidinyl, etc.; X, Y = independently O, S, NH; R = (un)substituted alk(en)yl, cycloalk(en)yl, hetero/arylalkyl, etc.; R1 = OH and derivs., OPO3H and derivs., OSO2H and derivs., etc.; R2 = H; R3 = halo/alkyl, halo/alkenyl, (un)substituted cycloalk(en)yl, aryl; R4 = (un)substituted cycloalk(en)yl, heterocyclyl, hetero/aryl] were prepared as HIV protease inhibitors. For example, II was prepared, in 62% yield, by coupling acid III (preparation given) with amine IV (preparation given). I showed antiviral activity against Wild-Type HIV with EC50 in the range of 1 nM to 100 nM.

IT **854742-03-3P 854742-27-1P 854742-66-8P 854742-68-0P 854742-79-3P 854742-80-6P 854746-70-6P 854746-71-7P 854746-72-8P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(antiviral agent; preparation of HIV protease inhibitors, in particular imidazolidine derivs.)

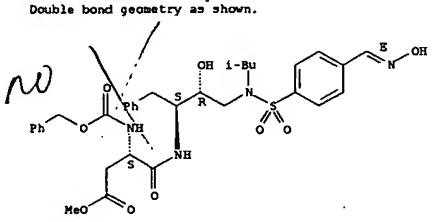
RN 854742-03-3 CAPLUS
CN INDEX NAME NOT YET ASSIGNED

Absolute stereochemistry.
Double bond geometry as shown.



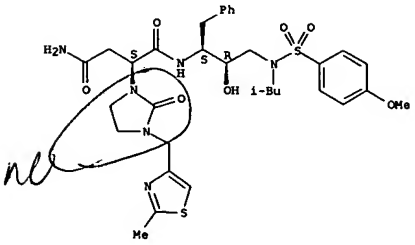
RN 854742-27-1 CAPLUS
CN INDEX NAME NOT YET ASSIGNED

Absolute stereochemistry.
Double bond geometry as shown.



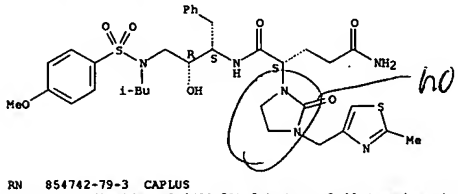
RN 854742-66-8 CAPLUS
CN Butanediamide, N1-[(1S,2R)-2-hydroxy-3-[[(4-methoxyphenyl)sulfonyl](2-methylpropyl)amino]-1-(phenylmethyl)propyl]-2-[3-[(2-methyl-4-thiazolyl)methyl]-2-oxo-1-imidazolidinyl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



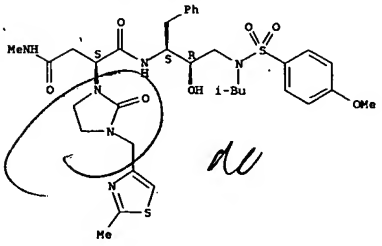
RN 854742-68-0 CAPLUS
CN Pentanediamide, N-[(1S,2R)-2-hydroxy-3-[[(4-methoxyphenyl)sulfonyl](2-methylpropyl)amino]-1-(phenylmethyl)propyl]-2-[3-[(2-methyl-4-thiazolyl)methyl]-2-oxo-1-imidazolidinyl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



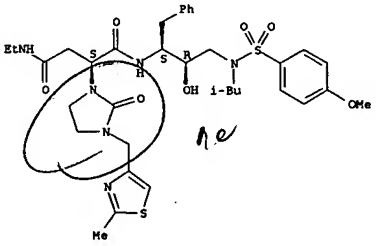
RN 854742-79-3 CAPLUS
CN Butanediamide, N1-[(1S,2R)-2-hydroxy-3-[[(4-methoxyphenyl)sulfonyl](2-methylpropyl)amino]-1-(phenylmethyl)propyl]-N4-methyl-2-[3-[(2-methyl-4-thiazolyl)methyl]-2-oxo-1-imidazolidinyl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 854742-80-6 CAPLUS
CN Butanediamide, N4-ethyl-N1-[(1S,2R)-2-hydroxy-3-[[(4-methoxyphenyl)sulfonyl](2-methylpropyl)amino]-1-(phenylmethyl)propyl]-2-[3-[(2-methyl-4-thiazolyl)methyl]-2-oxo-1-imidazolidinyl]-, (2S)- (9CI) (CA INDEX NAME)

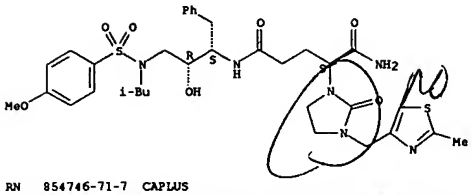
Absolute stereochemistry.



RN 854746-70-6 CAPLUS
CN Pentanediamide, N5-[(1S,2R)-2-hydroxy-3-[[(4-methoxyphenyl)sulfonyl](2-methylpropyl)amino]-1-(phenylmethyl)propyl]-2-[3-[(2-methyl-4-thiazolyl)methyl]-2-oxo-1-imidazolidinyl]-, (2S)- (9CI) (CA INDEX NAME)

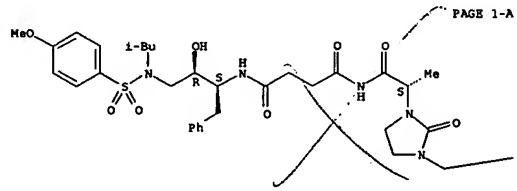
Absolute stereochemistry.

L4 ANSWER 1 OF 23 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



RN 854746-71-7 CAPLUS
CN Butanediamide, N-[(1S,2R)-2-hydroxy-3-[[(4-methoxyphenyl)sulfonyl](2-methylpropyl)amino]-1-(phenylmethyl)propyl]-N'-[(2S)-2-[3-[(2-methyl-5-thiazolyl)methyl]-2-oxo-1-imidazolidinyl]-1-oxopropyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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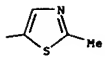
PAGE 1-B



RN 854746-72-8 CAPLUS
CN Butanediamide, N-[(1S,2R)-2-hydroxy-3-[[(4-methoxyphenyl)sulfonyl](2-methylpropyl)amino]-1-(phenylmethyl)propyl]-N'-[(2S)-2-[3-[(2-methyl-5-thiazolyl)methyl]-2-oxo-1-imidazolidinyl]-1-oxobutyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 2 OF 23 CAPLUS COPYRIGHT 2005 ACS on STN

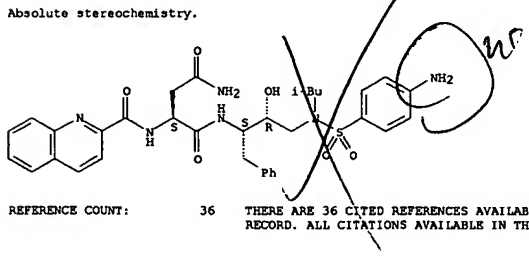
ACCESSION NUMBER: 2004:322087 CAPLUS
DOCUMENT NUMBER: 140:399222
TITLE: BREED: Generating Novel Inhibitors through Hybridization of Known Ligands. Application to CDK2, P38, and HIV Protease
AUTHOR(S): Pierce, Albert C.; Rao, Govinda; Bemis, Guy W.
CORPORATE SOURCE: Vertex Pharmaceuticals, Cambridge, MA, 02139, USA
SOURCE: Journal of Medicinal Chemistry (2004), 47(11), 2768-2775
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB In this work we describe BREED, a method for the generation of novel inhibitors from structures of known ligands bound to a common target. The method is essentially an automation of the common medicinal chemical practice of joining fragments of two known ligands to generate a new inhibitor. The ligand-bound target structures are overlaid, all overlapping bonds in all pairs of ligands are found, and the fragments on each side of each matching bond are swapped to generate the new mols. Since the method is automated, it can be applied recursively to generate all possible combinations of known ligands. In an application of this method to HIV protease inhibitors and protein kinase inhibitors, hundreds of new mol. structures were generated. These included known inhibitor scaffolds not included in the initial set, entirely novel scaffolds, and novel substituents on known scaffolds. The method is fast, and since all of the ligand functional groups are known to bind the target in the precise position and orientation present in the novel ligand, the success rate of this method should be superior to more traditional de novo design techniques. In an era of increasingly high-throughput structural biol., such methods for high-throughput utilization of structural information will become increasingly valuable.

IT 688359-10-6
RL: BSU (Biological study, unclassified); BIOL (Biological study) (novel method BREED for generating novel inhibitors through bond-matching and fragment swapping of known ligands)

RN 688359-10-6 CAPLUS
CN Butanediamide, N1-[(1S,2R)-3-[[(4-aminophenyl)sulfonyl](2-methylpropyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 1 OF 23 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

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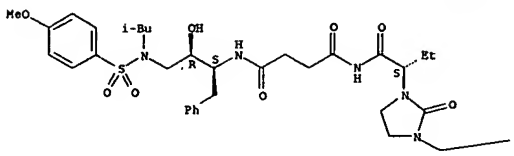

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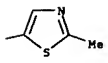
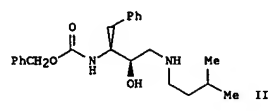


L4 ANSWER 3 OF 23 CAPLUS COPYRIGHT 2005 ACS on STN

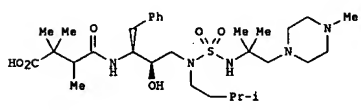
ACCESSION NUMBER: 2002:23862 CAPLUS
DOCUMENT NUMBER: 136:85665
TITLE: Succinoylamino hydroxyethylamino sulfonyl urea derivatives useful as retroviral protease inhibitors
INVENTOR(S): Vazquez, Michael L.; Mueller, Richard A.; Talley, John J.; Getman, Daniel P.; Decrescenzo, Gary A.; Sun, Eric T.
PATENT ASSIGNEE(S): G.D. Searle and Co., USA
SOURCE: U.S., 32 pp., Cont. of U.S. Ser. No. 219,048, abandoned.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6337398	B1	20020108	US 1995-542861	19951013
US 2002198378	A1	20021226	US 2001-11778	20011211
US 6515024	B2	20030204		
US 2004002542	A1	20040101	US 2002-315254	20021210
PRIORITY APPLN. INFO.:			US 1992-969682	B1 19921030
			US 1994-219048	B1 19940328
			US 1995-542861	A3 19951013
			US 2001-11778	A1 20011211

OTHER SOURCE(S): MARPAT 136:85665
GI



II



III

AB Intermediates used for the synthesis of title compds. R33R34X'-C:Y'-(CH2)pCR31R32-CR30R1-C:Y-NR6CHR2CHOHCH2NR3S(O)xNR4CR7R7'(CH2)nR8 [R1 = H, CH2SO2NH2, ester, amide, etc.; R2 = alkyl, aryl, cycloalkyl, etc.; R3 = (halo)alkyl, alken(yn)yl, hydroxyalkyl, etc.; R4 = H, R3; R6 = H, alkyl; R7-7' = H, R3, amino acid sidechains, etc.; R8 = CN, OH, alkyl, alkoxy, cycloalkyl, etc.; R30-32 = R1 or one of which combines with R1 to form a cycloalkyl radical; R33-34 = H, R1 or together with X' form a cycloalkyl

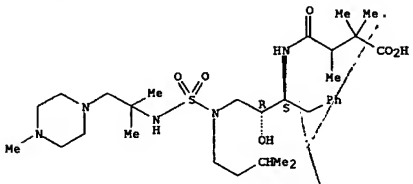
L4 ANSWER 3 OF 23 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
radical; x = 1 - 2; X' = N, O, CR17, where R17 = H, alkyl; n = 0 - 6; p = 0 - 2; Y, Y' = O, S, NR15, where R15 = H, R3; I] were prepd. For example, N-Cbz-L-phenylalanine chloromethyl ketone was reduced (MeOH/THF, -2°C, NaBH4), treated with base (EtOH, KOH) and the resulting epoxide intermediate reacted with isoamylamine (i-PrOH, reflux, 1.5 h) to give homochiral amine II in 31% yield for the 3 steps. II was elaborated by reaction with sulfamoyl chlorides/sulfamates, deprotected and functionalized with succinates to provide compds. I, e.g. claimed compd. III. I are effective as retroviral protease inhibitors, and in particular as inhibitors of HIV protease.

IT **386722-34-5P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug; succinoylamino hydroxyethylamino sulfonyl urea derivs. useful as retroviral protease inhibitors)

RN 386722-34-5 CAPLUS

CN 4-Thia-3,5,9-triazatridecan-13-oic acid, 7-hydroxy-2,2,11,12,12-pentamethyl-5-(3-methylbutyl)-1-(4-methyl-1-piperazinyl)-10-oxo-8-(phenylmethyl)-, 4,4-dioxide, (7R,8S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 49 THERE ARE 49 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 23 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2000:304314 CAPLUS
DOCUMENT NUMBER: 132:322147
TITLE: Preparation of α- and β-amino acid hydroxyethylamino sulfonamides as retro viral protease inhibitors.
INVENTOR(S): Vazquez, Michael L.; Mueller, Richard A.; Talley, John J.; Getman, Daniel P.; Decrescenzo, Gary A.; Freskos, John N.; Heintz, Robert M.; Bertenshaw, Deborah E.
PATENT ASSIGNEE(S): G.D.Searle and Co., USA
SOURCE: U.S., 93 pp., Cont.-in-part of Appl. PCT/US93/07814. CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 6
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6060476	A	20000509	US 1994-204827	19940302
WO 9404492	A1	19940303	WO 1993-US7814	19930824
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RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
EP 810209	A2	19971203	EP 1997-113434	19930824
EP 810209	A3	19981202		
EP 810209	B1	20020605		
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WO 9506030	A1	19950302	WO 1994-US9139	19940822
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RW: KE, MW, SD, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
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EP 715618	A1	19960612	EP 1994-927162	19940823
EP 715618	B1	19981216		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
AT 174587	E	19990115	AT 1994-927162	19940823
ES 2127938	T3	19990501	ES 1994-927162	19940823
US 5968942	A	19991019	US 1994-294468	19940823
US 6455581	B1	20020924	US 1995-451090	19950525
US 6248775	B1	20010619	US 1999-288080	19990408
US 6500832	B1	20021231	US 2000-525161	20000314
US 2002052399	A1	20020502	US 2001-798255	20010305
US 6417387	B2	20020709		
US 2003191319	A1	20031009	US 2002-157019	20020530
US 6646010	B2	20031111		
US 2004044047	A1	20040304	US 2002-199481	20020722
US 6846954	B2	20050125		
US 6924286	B1	20050802	US 2003-633376	20030804
US 2004229922	A1	20041118	US 2004-812343	20040330

PRIORITY APPLN. INFO.:

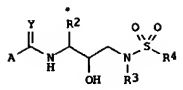
US 1992-934984	B2	19920825
WO 1993-US7814	A2	19930824
EP 1993-923714	A3	19930824
US 1993-110911	A	19930824
US 1994-204827	A	19940302
US 1994-294468	A1	19940823

L4 ANSWER 4 OF 23 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

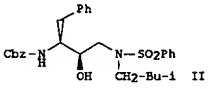
WO 1994-US9139	W	19940823
US 1995-451090	A3	19950525
US 1999-288080	A1	19990408
US 2001-798255	A1	20010305
US 2002-157019	A1	20020530
US 2002-199481	A3	20020722

OTHER SOURCE(S): MARPAT 132:322147

GI



I



II

AB Amino acid hydroxyethylamino sulfonamide compds. I [R2 = (un)substituted aryl, (cyclo)alkyl, aralkyl, cycloalkylalkyl; R3 = alkyl, haloalkyl, alkenyl, alkynyl, hydroxy-, alkoxy-, alkylthio-, or alkylsulfonylalkyl, cycloalkylalkyl, heterocycloalkyl, heteroaryl, heterocycloalkylalkyl, aryl, aralkyl, or heteroaralkyl; R4 = heterocycloalkyl, heteroaryl or aryl; Y = O or S; A = heterocycloalkyl, heterocycloalkoxy, heterocycloalkylalkoxy, heteroaralkyl, heteroarylalkoxy, heteroaryloxy or heteroaryl] were prepared as retroviral protease inhibitors, particular as inhibitors of HIV protease. Thus, compound II (Cbz = benzyloxycarbonyl) was prepared and assayed for HIV inhibitory activity (IC50 = 16 nM). Compds. of formula I were tested for cytotoxicity and efficacy (IC50, EC50 and TD50 values at the nanomolar level are tabulated).

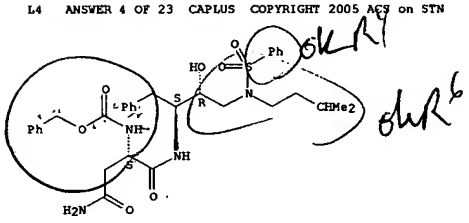
IT **159005-92-2P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(amino acid hydroxyethylamino sulfonamides as retroviral protease inhibitors)

RN 159005-92-2 CAPLUS

CN Carbamic acid, [(1S)-3-amino-1-[[[(1S,2R)-2-hydroxy-3-[(3-methylbutyl)(phenylsulfonyl)amino]-1-(phenylmethyl)propyl]amino]carbonyl]-3-oxopropyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 4 OF 23 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

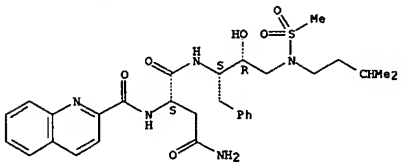


IT **159005-89-7P 159005-91-1P 159005-95-5P**
159006-21-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(amino acid hydroxyethylamino sulfonamides as retroviral protease inhibitors)

RN 159005-89-7 CAPLUS

CN Butanediamide, N1-[(1S,2R)-2-hydroxy-3-[(3-methylbutyl)(methylsulfonyl)amino]-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

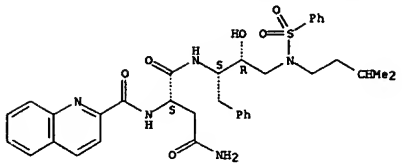


RN 159005-91-1 CAPLUS

CN Butanediamide, N1-[(1S,2R)-2-hydroxy-3-[(3-methylbutyl)(phenylsulfonyl)amino]-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

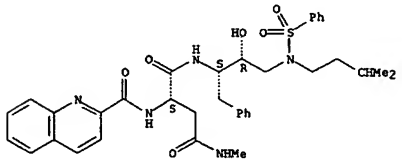
Absolute stereochemistry.

L4 ANSWER 4 OF 23 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



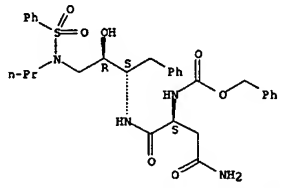
RN 159005-95-5 CAPLUS
CN Butanediamide, N1-[(1S,2R)-2-hydroxy-3-[(3-methylbutyl)(phenylsulfonyl)amino]-1-(phenylmethyl)propyl]-N4-methyl-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



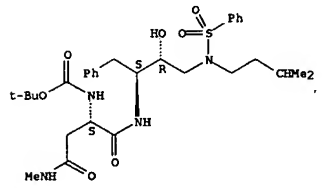
RN 159006-21-0 CAPLUS
CN Carbamic acid, [(1S)-3-amino-1-[[[(1S,2R)-2-hydroxy-1-(phenylmethyl)-3-[(phenylsulfonyl)propylamino]propyl]amino]carbonyl]-3-oxopropyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **159005-90-0P 159006-05-0P 159006-22-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(amino acid hydroxyethylamino sulfonamides as retroviral protease

L4 ANSWER 4 OF 23 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

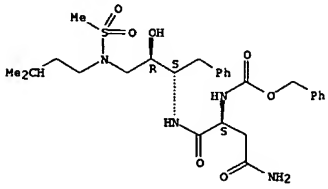


REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 23 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
inhibitors)

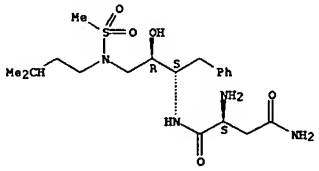
RN 159005-90-0 CAPLUS
CN 2-Thia-3,7,10-triazaundecan-11-oic acid, 9-(2-amino-2-oxoethyl)-5-hydroxy-3-(3-methylbutyl)-8-oxo-6-(phenylmethyl)-, phenylmethyl ester, 2,2-dioxide, (5R,6S,9S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 159006-05-0 CAPLUS
CN Butanediamide, 2-amino-N1-[(1S,2R)-2-hydroxy-3-[(3-methylbutyl)(methylsulfonyl)amino]-1-(phenylmethyl)propyl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 159006-22-1 CAPLUS
CN Carbamic acid, [(1S)-1-[[[(1S,2R)-2-hydroxy-3-[(3-methylbutyl)(phenylsulfonyl)amino]-1-(phenylmethyl)propyl]amino]carbonyl]-3-(methylamino)-3-oxopropyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 5 OF 23 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2000:220728 CAPLUS
DOCUMENT NUMBER: 132:265504
TITLE: Preparation of hydroxyethylamino sulfonamides useful as retroviral protease inhibitors.
INVENTOR(S): Vazquez, Michael L.; Mueller, Richard A.; Talley, John J.; Getman, Daniel P.; Decrescenzo, Gary A.; Freskos, John N.; Bertebshaw, Deborah E.; Heintz, Robert M.
PATENT ASSIGNEE(S): G.D. Searle and Co., USA
SOURCE: U.S., 119 pp., Cont.-in-part of U.S. 204,872, abandoned.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 6
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6046190	A	20000404	US 1996-586866	19960124
WO 9404492	A1	19940303	WO 1993-US7814	19930824
W: AT, AU, BB, BG, BR, BY, CA, CH, CZ, DE, DK, ES, FI, GB, HU, JP, KP, KR, KZ, LK, LU, MG, MN, MW, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SK, UA, US, VN				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
EP 810209	A2	19971203	EP 1997-113434	19930824
EP 810209	A3	19981202		
EP 810209	B1	20020605		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE				
WO 9506030	A1	19950302	WO 1994-US9139	19940823
W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, ES, FI, GB, GE, HU, JP, KE, KG, KP, KR, KZ, LK, LT, LU, LV, MD, MG, MN, MW, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SI, SK, TJ, TT, UA, US, US, UZ, VN				
RW: KE, MW, SD, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				

PRIORITY APPLN. INFO.:
US 1992-934984 B2 19920825
WO 1993-US7814 A2 19930824
US 1994-204872 B2 19940302
WO 1994-US9139 W 19940823
EP 1993-923714 A3 19930824
US 1993-110911 A 19930824
US 1994-204827 A 19940302

OTHER SOURCE(S): MARPAT 132:265504

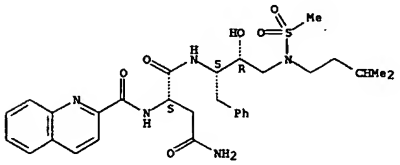
AB Hydroxyethylamino sulfonamide compds. R9R10N(CR7R8)pCHR1C(:Y)NR6CHR2CH(OH)CH2NR3S(:O)xR4 [I: R1 = H, CH2SO2NH2, CH2CO2CH3, alkyl, haloalkyl, alkenyl, alkynyl, cycloalkyl, amino acid side chains, etc.; R2 = (un)substituted alkyl, aryl, cycloalkyl, cycloalkylalkyl, aralkyl; R3 = H, alkyl, haloalkyl, alkenyl, alkynyl, aryl, heteroaryl, mono- and disubstituted aminoalkyl, etc.; R4 = alkyl, haloalkyl, alkenyl, alkynyl, aryl, (un)saturated heterocycle, (un)substituted aromatic heterocycloalkyl, etc.; R6 = H, alkyl; Y = O, S, NR3; R7,R8 = independently H, R1, or together with R1 and the carbon atoms to which they are attached represent a cycloalkyl radical; R9 = H, R3, or R3SO2; R10 = H, alkoxycarbonyl, alkylcarbonyl, aroyl, aryloxycarbonyl, heterocyclylalkoxycarbonyl, mono- and disubstituted aminocarbonyl, or aminoalkanoyl, etc.; or R9R10N = heterocycloalkyl or heteroaryl; x = 0-2; p = 0-1] or their pharmaceutically acceptable salts, prodrugs, or esters were prepared as inhibitors of retroviral proteases such as human immunodeficiency virus

(HIV). Many inhibitors were prepd. by (1) prepg. an N-protected amino epoxide and (2) reacting this with an amine and (3) prepg. a sulfonamide by reacting with a sulfonyl chloride or sulfonyl anhydride in the presence of an acid scavenger. The amino function of the sulfonamide was then (4) deprotected and (5) reacted with a carboxylate. Thus, N1-[2R-hydroxy-3-[(3-methylbutyl)(phenylsulfonyl)amino]-1S-(phenylmethyl)propyl]-2S-[(2-quinolinylcarbonyl)amino]butanediamide was prepd. and assayed for HIV protease inhibitory activity (IC50 = 1.5 nM). Compds. of formula I were tested for cytotoxicity and antiviral efficacy (IC50, EC50, and TD50 values at the nanomolar level are tabulated).

IT 159005-89-7P 159005-91-1P 159005-92-2P
159005-95-5P 159006-21-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of hydroxyethylamino sulfonamides useful as retroviral protease
inhibitors)

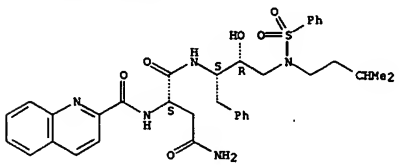
RN 159005-89-7 CAPLUS
CN Butanediamide, N1-[(1S,2R)-2-hydroxy-3-[(3-methylbutyl)(methylsulfonyl)amino]-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 159005-91-1 CAPLUS
CN Butanediamide, N1-[(1S,2R)-2-hydroxy-3-[(3-methylbutyl)(phenylsulfonyl)amino]-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

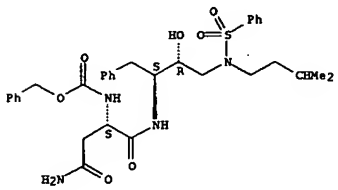
Absolute stereochemistry.



RN 159005-92-2 CAPLUS
CN Carbamic acid, [(1S)-3-amino-1-[[[(1S,2R)-2-hydroxy-3-[(3-

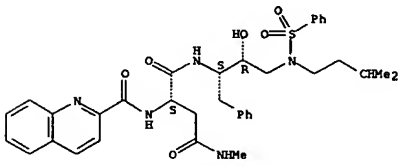
methylbutyl)(phenylsulfonyl)amino]-1-(phenylmethyl)propyl]amino]carbonyl]-3-oxopropyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



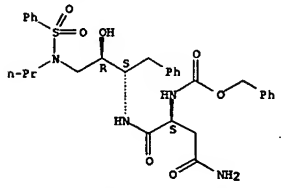
RN 159005-95-5 CAPLUS
CN Butanediamide, N1-[(1S,2R)-2-hydroxy-3-[(3-methylbutyl)(phenylsulfonyl)amino]-1-(phenylmethyl)propyl]-N4-methyl-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 159006-21-0 CAPLUS
CN Carbamic acid, [(1S)-3-amino-1-[[[(1S,2R)-2-hydroxy-1-(phenylmethyl)-3-[(phenylsulfonyl)propylamino]propyl]amino]carbonyl]-3-oxopropyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

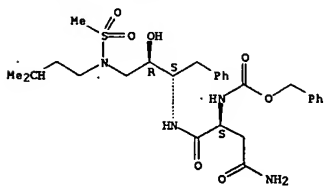
Absolute stereochemistry.



IT 159005-90-0P 159006-05-0P 159006-06-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of hydroxyethylamino sulfonamides useful as retroviral protease
inhibitors)

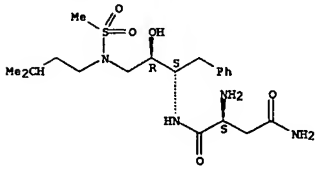
RN 159005-90-0 CAPLUS
CN 2-Thia-3,7,10-triazaundecan-11-oic acid, 9-(2-amino-2-oxoethyl)-5-hydroxy-3-(3-methylbutyl)-8-oxo-6-(phenylmethyl)-, phenylmethyl ester, 2,2-dioxide, (5R,6S,9S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



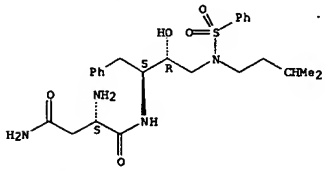
RN 159006-05-0 CAPLUS
CN Butanediamide, 2-amino-N1-[(1S,2R)-2-hydroxy-3-[(3-methylbutyl)(methylsulfonyl)amino]-1-(phenylmethyl)propyl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 159006-06-1 CAPLUS
CN Butanediamide, 2-amino-N1-[(1S,2R)-2-hydroxy-3-[(3-methylbutyl)(phenylsulfonyl)amino]-1-(phenylmethyl)propyl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 45 THERE ARE 45 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 6 OF 23 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1999:811207 CAPLUS
DOCUMENT NUMBER: 132:49801
TITLE: Preparation of 1-acylamino-3-(N-arylsulfonyl-N-alkoxyamino)-2-hydroxypropanes and related compounds as inhibitors of HIV aspartyl protease.
INVENTOR(S): Sherrill, Ronald George; Hale, Michael R.; Spaltenstein, Andrew; Furfine, Eric Steven; Andrews, Clarence Webster, III; Lowen, Gregory Thomas
PATENT ASSIGNEE(S): Vertex Pharmaceuticals Incorporated, USA
SOURCE: PCT Int. Appl., 344 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9965870	A2	19991223	WO 1999-US13744	19990617
WO 9965870	A3	20010315		
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2335477	AA	19991223	CA 1999-2335477	19990617
AU 9945760	A1	20000105	AU 1999-45760	19990617
AU 767728	B2	20031120		
EP 1086076	A1	20010328	EP 1999-928769	19990617
EP 1086076	B1	20041222		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
BR 9912169	A	20010410	BR 1999-12169	19990617
NZ 508855	A	20031031	NZ 1999-508855	19990617
AT 285396	E	20050115	AT 1999-928769	19990617
ES 2235492	T3	20050701	ES 1999-928769	19990617
US 2002049201	A1	20020425	US 2000-731129	20001206
US 6613743	B2	20030902		
NO 2000006405	A	20010219	NO 2000-6405	20001215
US 2004097594	A1	20040520	US 2003-600937	20030620
NZ 528074	A	20041126	NZ 2003-528074	20030908

PRIORITY APPLN. INFO.: US 1998-90094P P 19980619
WO 1999-US13744 W 19990617
US 2000-731129 A3 20001206

OTHER SOURCE(S): MARPAT 132:49801

AB ABxN(Gx)CHDCHOR7CH2ND'SO2E [A = H, (substituted) Ht, R1Ht, R1Ak; Ak = alkyl; Ht = cycloalkyl, cycloalkenyl, (substituted) aryl, heterocyclyl; R1 = CO, SO2, COCO, O2C, NR2CO, NR2SO2, etc.; B = null, NR2C(R3)2CO; x = 0, 1; R2 = H, (substituted) Ht, alkyl; R3 = H, (substituted) Ht, alkyl, alkenyl, cycloalkyl, cycloalkenyl; G = null, H, R7, alkyl; G may be bound to R7; D = (substituted) Q, alkyl, alkenyl; Q = (substituted) carbocyclyl, heterocyclyl; D' = OR10, N:R10, N(R10)R1R3; E = Ht, OHt, OR3, NR2R3, (substituted) alkyl, alkenyl, etc.; R7 = H, (CH2O)xY(ZM)(:X)Z(M)x, etc.; M = null, H, Li, Na, K, Mg, Ca, Ba, alkyl, alkenyl, etc.; X = O, S; Y = P, S; Z = O, S, N(R2)2, H], were prepared as inhibitors of HIV aspartyl protease (no data). Thus, 3-H2NC6H4SO2NHOCHMe2 (preparation given), tert-Bu

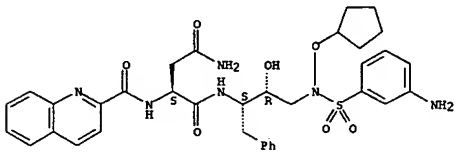
L4 ANSWER 6 OF 23 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

N-(1S)-1-[(2S)-oxiran-2-yl]-2-phenylethylcarbamate, and phosphazene base P4 tert-Bu were stirred in 8 h in THF to give 95% tert-Bu N-(1S,2R)-3-[[(3-aminophenyl)sulfonyl](isopropoxy)amino]-1-benzyl-2-hydroxypropylcarbamate.

IT 252871-32-2P 252871-33-3P 252871-34-4P 252871-35-5P 252871-52-6P 252871-57-1P 252871-63-9P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 1-acylamino-3-(N-arylsulfonyl-N-alkoxyamino)-2-hydroxypropanes and related compds. as inhibitors of HIV aspartyl protease)

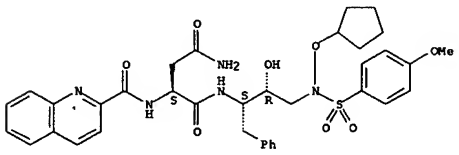
RN 252871-32-2 CAPLUS
CN Butanediamide, N1-[(1S,2R)-3-[[(3-aminophenyl)sulfonyl](cyclopentyloxy)amino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 252871-33-3 CAPLUS
CN Butanediamide, N1-[(1S,2R)-3-[(cyclopentyloxy)[(4-methoxyphenyl)sulfonyl]amino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

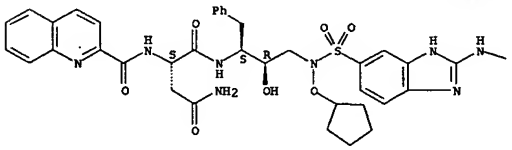


RN 252871-34-4 CAPLUS
CN Carbamic acid, [5-[[[(2R,3S)-3-[[(2S)-4-amino-1,4-dioxo-2-[(2-quinolinylcarbonyl)amino]butyl]amino]-2-hydroxy-4-phenylbutyl](cyclopentyloxy)amino]sulfonyl]-1H-benzimidazol-2-yl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 6 OF 23 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

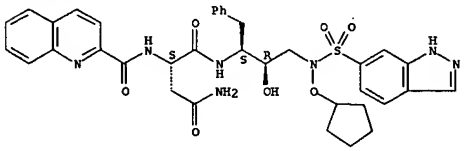
PAGE 1-A



PAGE 1-B

RN 252871-35-5 CAPLUS
CN Butanediamide, N1-[(1S,2R)-3-[(cyclopentyloxy)(1H-indazol-6-ylsulfonyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

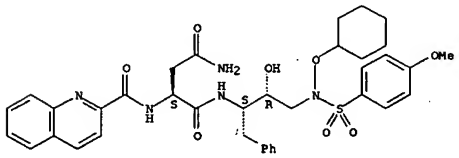
Absolute stereochemistry.



RN 252871-52-6 CAPLUS
CN Butanediamide, N1-[(1S,2R)-3-[(cyclohexyloxy)[(4-methoxyphenyl)sulfonyl]amino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

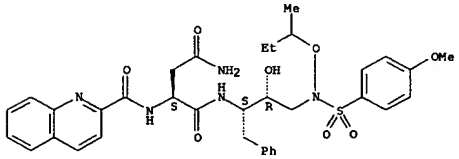
Absolute stereochemistry.

L4 ANSWER 6 OF 23 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



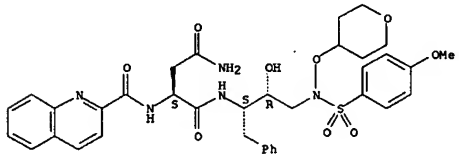
RN 252871-57-1 CAPLUS
CN Butanediamide, N1-[(1S,2R)-2-hydroxy-3-[[(4-methoxyphenyl)sulfonyl](1-methylpropoxy)amino]-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 252871-63-9 CAPLUS
CN Butanediamide, N1-[(1S,2R)-2-hydroxy-3-[[(4-methoxyphenyl)sulfonyl][(tetrahydro-2H-pyran-4-yl)oxy]amino]-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 7 OF 23 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1999:670116 CAPLUS
DOCUMENT NUMBER: 131:295568
TITLE: α- and β-Amino acid hydroxyethylamino sulfonamides useful as retroviral protease inhibitors
INVENTOR(S): Vazques, Michael L.; Mueller, Richard A.; Talley, John J.; Getman, Daniel P.; Decrescenzo, Gary A.; Freskos, John N.; Bertenshaw, Deborah E.; Heintz, Robert M.
PATENT ASSIGNEE(S): G. D. Searle and Co., USA
SOURCE: U.S., 130 pp., Cont.-in-part of U. S. 204,827.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 6
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5968942	A	19991019	US 1994-294468	19940823
WO 9404492	A1	19940303	WO 1993-US7814	19930824
W: AT, AU, BB, BG, BR, BY, CA, CH, CZ, DE, DK, ES, FI, GB, HU, JP, KP, KR, KZ, LK, LU, MG, MN, MW, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SK, UA, US, VN				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
EP 810209	A2	19971203	EP 1997-113434	19930824
EP 810209	A3	19981202		
EP 810209	B1	20020605		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE				
US 6060476	A	20000509	US 1994-204827	19940302
US 6248775	B1	20010619	US 1999-288080	19990408
US 2002052399	A1	20020502	US 2001-798255	20010305
US 6417387	B2	20020709		
US 2003191319	A1	20031009	US 2002-157019	20020530
US 6646010	B2	20031111		
US 6924286	B1	20050802	US 2003-633376	20030804

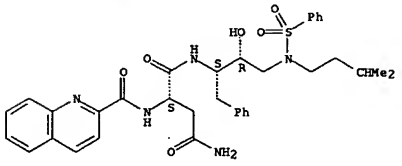
PRIORITY APPLN. INFO.:
US 1992-934984 B2 19920825
WO 1993-US7814 A2 19930824
US 1994-204827 A2 19940302
EP 1993-923714 A3 19930824
US 1993-110911 A2 19930824
US 1994-294468 A1 19940823
US 1999-288080 A1 19990408
US 2001-798255 A1 20010305
US 2002-157019 A1 20020530

OTHER SOURCE(S): MARPAT 131:295568

AB α- And β-Amino acid hydroxyethylamino sulfonamide compds. are effective as retroviral protease inhibitors, and in particular as inhibitors of HIV protease, as well as effective in preventing the growth of retroviruses in a solution General and specific schemes for chemical synthesis of the sulfonamide-containing hydroxyethylamine inhibitor compds. are described. Seventy-eight such compds. were tested for cytotoxicity and antiviral efficacy (IC50, EC50, and TD50 values at the nanomolar level are tabulated).

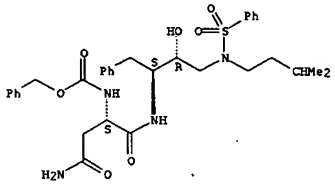
IT **159005-89-7P 159005-90-0P 159005-91-1P**
159005-92-2P 159005-95-5P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(α- and β-amino acid hydroxyethylamino sulfonamides useful as retroviral protease inhibitors)

L4 ANSWER 7 OF 23 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



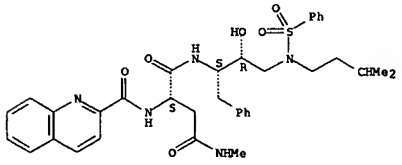
RN 159005-92-2 CAPLUS
CN Carbamic acid, [(1S)-3-amino-1-[[[(1S,2R)-2-hydroxy-3-[(3-methylbutyl)(phenylsulfonyl)amino]-1-(phenylmethyl)propyl]amino]carbonyl]-3-oxopropyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 159005-95-5 CAPLUS
CN Butanediamide, N1-[(1S,2R)-2-hydroxy-3-[(3-methylbutyl)(phenylsulfonyl)amino]-1-(phenylmethyl)propyl]-N4-methyl-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

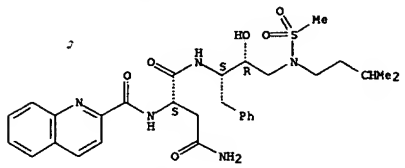


IT **159006-21-0P 159006-22-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(α- and β-amino acid hydroxyethylamino sulfonamides useful

L4 ANSWER 7 OF 23 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

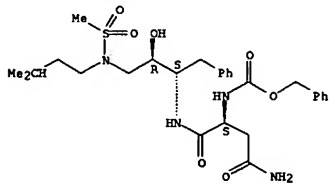
RN 159005-89-7 CAPLUS
CN Butanediamide, N1-[(1S,2R)-2-hydroxy-3-[(3-methylbutyl)(methylsulfonyl)amino]-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 159005-90-0 CAPLUS
CN 2-Thia-3,7,10-triazaundecan-11-oic acid, 9-(2-amino-2-oxoethyl)-5-hydroxy-3-(3-methylbutyl)-8-oxo-6-(phenylmethyl)-, phenylmethyl ester, 2,2-dioxide, (5R,6S,9S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



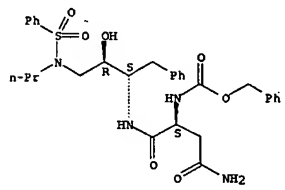
RN 159005-91-1 CAPLUS
CN Butanediamide, N1-[(1S,2R)-2-hydroxy-3-[(3-methylbutyl)(phenylsulfonyl)amino]-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 7 OF 23 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
as retroviral protease inhibitors)

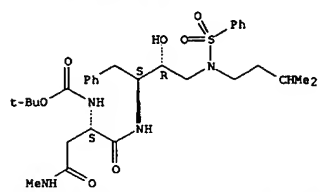
RN 159006-21-0 CAPLUS
CN Carbamic acid, [(1S)-3-amino-1-[[[(1S,2R)-2-hydroxy-1-(phenylmethyl)-3-[(phenylsulfonyl)propylamino]propyl]amino]carbonyl]-3-oxopropyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 159006-22-1 CAPLUS
CN Carbamic acid, [(1S)-1-[[[(1S,2R)-2-hydroxy-3-[(3-methylbutyl)(phenylsulfonyl)amino]-1-(phenylmethyl)propyl]amino]carbonyl]-3-(methylamino)-3-oxopropyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 8 OF 23 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1998:799692 CAPLUS
DOCUMENT NUMBER: 130:38712
TITLE: Preparation of α- and β-amino acid hydroxyethylamino sulfonamides useful as retroviral protease inhibitors
INVENTOR(S): Vazquez, Michael L.; Mueller, Richard A.; Talley, John J.; Getman, Daniel; Decrescenzo, Gary A.; Freskos, John N.
PATENT ASSIGNEE(S): G.D. Searle and Co., USA
SOURCE: U.S., 67 pp., Cont.-in-part of U.S. Ser. No. 934,984, abandoned.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 6
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5843946	A	19981201	US 1993-110911	19930824
EP 810209	A2	19971203	EP 1997-113434	19930824
EP 810209	A3	19981202		
EP 810209	B1	20020605		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE				
AT 172717	E	19981115	AT 1993-923714	19930824
ES 2123065	T3	19990101	ES 1993-923714	19930824
AT 218541	E	20020615	AT 1997-113434	19930824
PT 810209	T	20020930	PT 1997-113434	19930824
ES 2177868	T3	20021216	ES 1997-113434	19930824
WO 9506030	A1	19950302	WO 1994-US9139	19940823
W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, ES, FI, GB, GE, HU, JP, KE, KG, KP, KR, KZ, LK, LT, LU, LV, MD, MG, MN, MW, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SI, SK, TJ, TT, UA, US, US, UZ, VN				
RW: KE, MW, SD, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9476697	A1	19950321	AU 1994-76697	19940823
EP 715618	A1	19960612	EP 1994-927162	19940823
EP 715618	B1	19981216		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
AT 174587	E	19990115	AT 1994-927162	19940823
ES 2127938	T3	19990501	ES 1994-927162	19940823
FI 9500650	A	19950214	FI 1995-650	19950214
FI 112471	B1	20031215		
US 5786483	A	19980728	US 1995-487662	19950607
US 5830897	A	19981103	US 1995-473698	19950607
US 6172082	B1	20010109	US 1995-476788	19950607
US 5744481	A	19980428	US 1997-845392	19970425
US 6248775	B1	20010619	US 1999-288080	19990408
US 6335460	B1	20020101	US 2000-510189	20000222
US 6472407	B1	20021029	US 2000-511005	20000222
US 6534493	B1	20030318	US 2000-694785	20001024
US 2002052399	A1	20020502	US 2001-798255	20010305
US 6417387	B2	20020709		
US 2003191319	A1	20031009	US 2002-157019	20020530
US 6646010	B2	20031111		
US 6924286	B1	20050802	US 2003-633376	20030804
PRIORITY APPLN. INFO.:			US 1992-934984	B2 19920825
			EP 1993-923714	A3 19930824
			US 1993-110911	A 19930824

L4 ANSWER 8 OF 23 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

	WO 1993-US7814	A2 19930824
	US 1994-204827	A 19940302
	US 1994-294468	A1 19940823
	WO 1994-US9139	W 19940823
	US 1995-476788	A1 19950607
	US 1995-485524	B1 19950607
	US 1999-288080	A1 19990408
	US 2001-798255	A1 20010305
	US 2002-157019	A1 20020530

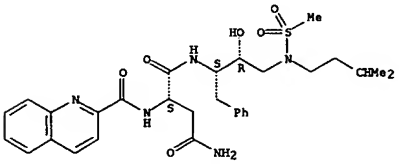
OTHER SOURCE(S): MARPAT 130:38712

AB Amino acid hydroxyethylamino sulfonamide compds. P1NHCHR2CH(OH)CH2NR3SO2R4 [P1 = alkoxycarbonyl, aralkoxycarbonyl, alkanoyl, cycloalkylcarbonyl, cycloalkylalkoxycarbonyl, cycloalkylalkanoyl, aralkanoyl, aroyl, aryloxycarbonyl, heterocyclylcarbonyl, heterocyclyloxycarbonyl, heterocyclylalkoxycarbonyl, heteroaralkoxycarbonyl, heteroaryloxycarbonyl, heteroaroyl; R2 = alkyl, aryl, cycloalkyl, cycloalkylalkyl, (un)substituted aralkyl; R3 = H, alkyl, alkenyl, alkynyl, hydroxyalkyl, alkoxyalkyl, cycloalkyl, cycloalkylalkyl, heterocyclyl, heteroaryl, heterocyclylalkyl, aryl, aralkyl, heteroaralkyl; R4 = alkyl, haloalkyl, alkenyl, alkynyl, cycloalkyl, heterocycloalkyl, heteroaryl, aryl, aralkyl] were preparation as retroviral protease inhibitors. Thus, N-[2R-hydroxy-3-[[(4-methoxyphenyl)sulfonyl](2-methylpropyl)amino]-1S-(phenylmethyl)propyl]-4-pyridinecarboxamide was prepared by amidation of isonicotinoyl chloride hydrochloride with 2R-hydroxy-3-[(2-methylpropyl)[(4-methoxyphenyl)sulfonyl]amino]-1S-(phenylmethyl)propylamine. Protease inhibitory data are tabulated.

IT **159005-89-7P 159005-91-1P 159005-92-2P**
159005-95-5P 159006-21-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of amino acid hydroxyethylamino sulfonamides useful as retroviral protease inhibitors)

RN 159005-89-7 CAPLUS
CN Butanediamide, N1-[(1S,2R)-2-hydroxy-3-[(3-methylbutyl)(methylsulfonyl)amino]-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

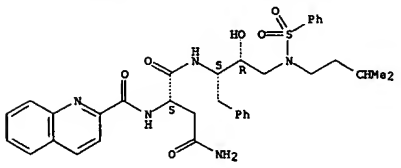
Absolute stereochemistry.



RN 159005-91-1 CAPLUS
CN Butanediamide, N1-[(1S,2R)-2-hydroxy-3-[(3-methylbutyl)(phenylsulfonyl)amino]-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

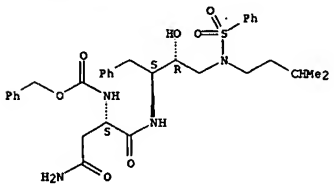
Absolute stereochemistry.

L4 ANSWER 8 OF 23 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



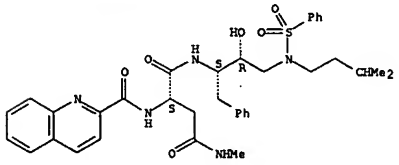
RN 159005-92-2 CAPLUS
CN Carbamic acid, [(1S)-3-amino-1-[[[(1S,2R)-2-hydroxy-3-[(3-methylbutyl)(phenylsulfonyl)amino]-1-(phenylmethyl)propyl]amino]carbonyl]-3-oxopropyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 159005-95-5 CAPLUS
CN Butanediamide, N1-[(1S,2R)-2-hydroxy-3-[(3-methylbutyl)(phenylsulfonyl)amino]-1-(phenylmethyl)propyl]-N4-methyl-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

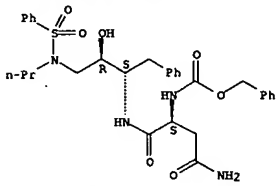
Absolute stereochemistry.



RN 159006-21-0 CAPLUS
CN Carbamic acid, [(1S)-3-amino-1-[[[(1S,2R)-2-hydroxy-1-(phenylmethyl)-3-[(phenylsulfonyl)propylamino]propyl]amino]carbonyl]-3-oxopropyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 8 OF 23 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

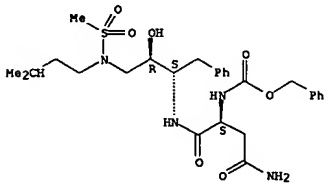
Absolute stereochemistry.



IT **159005-90-0P 159006-05-0P 159006-06-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of amino acid hydroxyethylamino sulfonamides useful as retroviral protease inhibitors)

RN 159005-90-0 CAPLUS
CN 2-Thia-3,7,10-triazaundecan-11-oic acid, 9-(2-amino-2-oxoethyl)-5-hydroxy-3-(3-methylbutyl)-8-oxo-6-(phenylmethyl)-, phenylmethyl ester, 2,2-dioxide, (5R,6S,9S)- (9CI) (CA INDEX NAME)

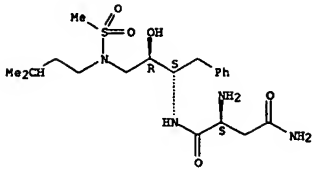
Absolute stereochemistry.



RN 159006-05-0 CAPLUS
CN Butanediamide, 2-amino-N1-[(1S,2R)-2-hydroxy-3-[(3-methylbutyl)(methylsulfonyl)amino]-1-(phenylmethyl)propyl]-, (2S)- (9CI) (CA INDEX NAME)

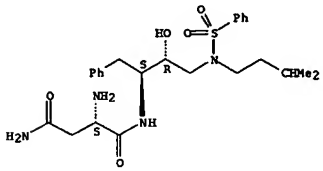
Absolute stereochemistry.

L4 ANSWER 8 OF 23 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



RN 159006-06-1 CAPLUS
CN Butanediamide, 2-amino-N1-[(1S,2R)-2-hydroxy-3-[(3-methylbutyl)(phenylsulfonyl)amino]-1-(phenylmethyl)propyl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



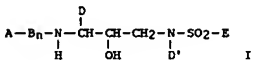
REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 9 OF 23 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1998:502547 CAPLUS
DOCUMENT NUMBER: 129:136097
TITLE: Preparation of heterocyclic sulfonamide inhibitors of aspartyl protease
INVENTOR(S): Tung, Roger D.; Murcko, Mark A.; Bhisetti, Govinda Rao
PATENT ASSIGNEE(S): Vertex Pharmaceuticals, Incorporated, USA
SOURCE: U.S., 87 pp., Cont.-in-part of U.S. 5,585,397.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 5
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5783701	A	19980721	US 1995-393460	19950223
EP 885887	A2	19981223	EP 1998-113921	19930907
EP 885887	A3	19990203		
EP 885887	B1	20030528		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE				
US 5585397	A	19961217	US 1993-142327	19931124
US 5723490	A	19980303	US 1995-424819	19950419
US 5977137	A	19991102	US 1998-115394	19980714
US 6392046	B1	20020521	US 1999-409808	19990930
US 2003064977	A1	20030403	US 2002-94763	20020308
US 6720335	B2	20040413		
US 2004167116	A1	20040826	US 2004-786997	20040224
PRIORITY APPLN. INFO.:			US 1992-941982	B2 19920908
			US 1993-142327	A2 19931124
			EP 1993-921428	A3 19930907
			WO 1993-US8458	W 19930907
			US 1995-393460	B2 19950223
			US 1998-115394	A3 19980714
			US 1999-409808	A3 19990930
			US 2002-94763	A1 20020308

OTHER SOURCE(S): MARPAT 129:136097
GI



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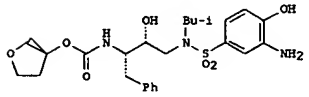


II

AB The title compds. I [A = H, -Ht, -R1Ht, (un)substituted -R1-alk(en)yl; R1 = CO, SO2, COCO, OCO, OSO2, NR2SO2, NR2CO, NR2COCO; Ht = (un)substituted

L4 ANSWER 9 OF 23 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

cycloalk(en)yl, aryl, (benzo)heterocyclyl; R2 = H, alkyl, -alkyl-R7; B = NR2C(R3)2CO; n = 0, 1; R3 = (un)substituted alk(en)yl or cycloalk(en)yl; n = 1, 2; D, D' = R7, (un)substituted alk(en)yl or cycloalk(en)yl; R7 = (un)substituted Ph, carbocyclyl, or heterocyclyl; E = Ht, -O-Ht, -Ht-Ht, OR3, NR2R3, (un)substituted alk(en)yl or carbocyclyl; R4 = OR2, CONHR2, SO2NHR2, halo, NR2COR2, cyano] are prepd. as inhibitors of HIV aspartyl protease. The invention also relates to pharmaceutical compns. comprising these compds. The compds. and pharmaceutical compns. are particularly well suited for inhibiting HIV-1 and HIV-2 protease activity. The invention also relates to methods for inhibiting the activity of HIV aspartyl protease using the invention compds., and to methods for screening compds. for anti-HIV activity. Prepns. of almost 200 compds. are described, and some of these plus addnl. compds. are claimed. Some of the compds., e.g., II, inhibit HIV replication (IC90) in CCRM-CEM cells in vitro at concns. of ≤ 100 nM.

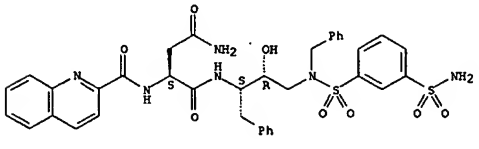
IT **186463-21-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of heterocyclic sulfonamide derivs. as inhibitors of HIV aspartyl protease)

RN 186463-21-8 CAPLUS
CN Butanediamide, N1-[(1S,2R)-3-[[[3-(aminosulfonyl)phenyl]sulfonyl](phenylmethyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)-, mono(trifluoroacetate) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 160230-14-8
CMF C37 H38 N6 O8 S2

Absolute stereochemistry.



CM 2

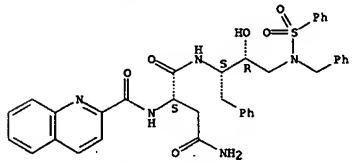
CRN 76-05-1
CMF C2 H F3 O2

L4 ANSWER 9 OF 23 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

IT **160230-05-7P 160230-06-8P 160230-07-9P**
160230-08-0P 160230-09-1P 160230-10-4P
160230-11-5P 160230-12-6P 160230-13-7P
160230-14-8P 160230-15-9P 160230-16-0P
160230-17-1P 160230-18-2P 160230-19-3P
160230-20-6P 160230-21-7P 160230-22-8P
160230-23-9P 160230-24-0P 160230-25-1P
160230-50-2P 160231-93-6P 160231-96-9P
160333-42-6P 160333-43-7P 160333-44-8P
160333-45-9P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of heterocyclic sulfonamide derivs. as inhibitors of HIV aspartyl protease)

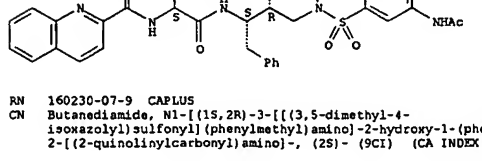
RN 160230-05-7 CAPLUS
CN Butanediamide, N1-[(1S,2R)-2-hydroxy-1-(phenylmethyl)-3-[(phenylmethyl)(phenylsulfonyl)amino]propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



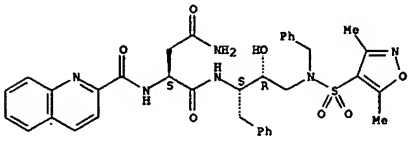
RN 160230-06-8 CAPLUS
CN Butanediamide, N1-[(1S,2R)-3-[[[3-(acetylamino)-4-fluorophenyl]sulfonyl](phenylmethyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



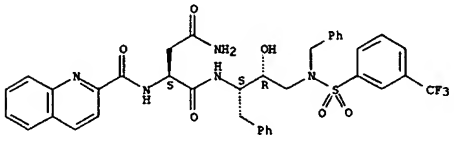
RN 160230-07-9 CAPLUS
CN Butanediamide, N1-[(1S,2R)-3-[[(3,5-dimethyl-4-isoxazolyl)sulfonyl](phenylmethyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



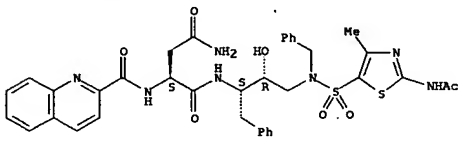
RN 160230-08-0 CAPLUS
CN Butanediamide, N1-[(1S,2R)-2-hydroxy-1-(phenylmethyl)-3-[(phenylmethyl)[[3-(trifluoromethyl)phenyl]sulfonyl]amino]propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



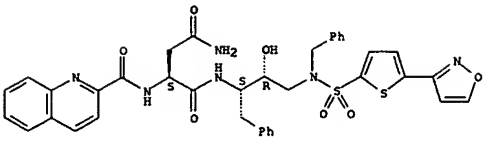
RN 160230-09-1 CAPLUS
CN Butanediamide, N1-[(1S,2R)-3-[[[2-(acetylamino)-4-methyl-5-thiazolyl]sulfonyl](phenylmethyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



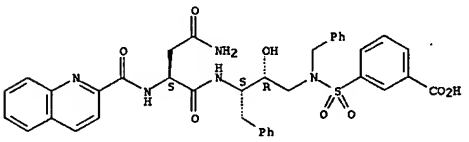
RN 160230-10-4 CAPLUS
CN Butanediamide, N1-[(1S,2R)-2-hydroxy-3-[[[5-(3-isoxazolyl)-2-thienyl]sulfonyl](phenylmethyl)amino]-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



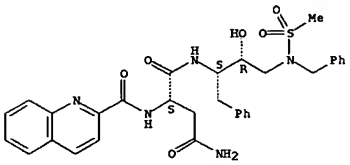
RN 160230-11-5 CAPLUS
CN Benzoic acid, 3-[[[(2R,3S)-3-[[(2S)-4-amino-1,4-dioxo-2-[(2-quinolinylcarbonyl)amino]butyl]amino]-2-hydroxy-4-phenylbutyl](phenylmethyl)amino]sulfonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



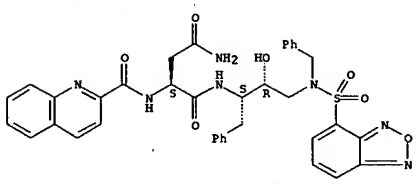
RN 160230-12-6 CAPLUS
CN Butanediamide, N1-[(1S,2R)-2-hydroxy-3-[(methylsulfonyl)(phenylmethyl)amino]-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



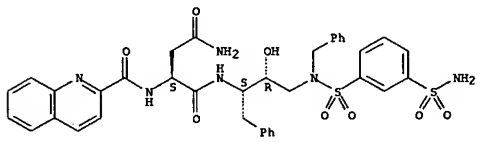
RN 160230-13-7 CAPLUS
CN Butanediamide, N1-[(1S,2R)-3-[(2,1,3-benzoxadiazol-4-ylsulfonyl)(phenylmethyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



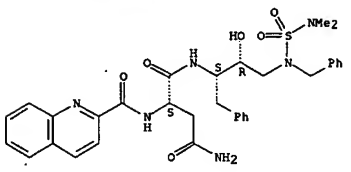
RN 160230-14-8 CAPLUS
CN Butanediamide, N1-[(1S,2R)-3-[[[3-(aminosulfonyl)phenyl]sulfonyl](phenylmethyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



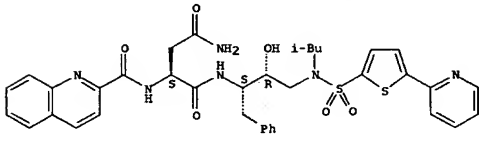
RN 160230-15-9 CAPLUS
CN Butanediamide, N1-[(1S,2R)-3-[[(dimethylamino)sulfonyl](phenylmethyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



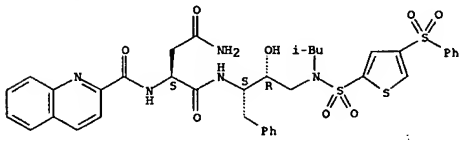
RN 160230-16-0 CAPLUS
CN Butanediamide, N1-[(1S,2R)-2-hydroxy-3-[(2-methylpropyl)[5-(2-pyridinyl)-2-thienyl]sulfonyl]amino]-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



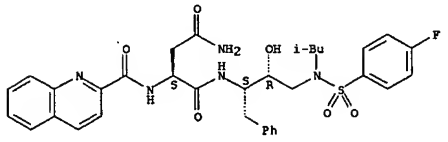
RN 160230-17-1 CAPLUS
CN Butanediamide, N1-[(1S,2R)-2-hydroxy-3-[(2-methylpropyl)[[4-(phenylsulfonyl)-2-thienyl]sulfonyl]amino]-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



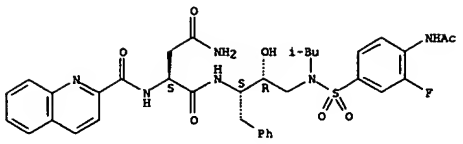
RN 160230-18-2 CAPLUS
CN Butanediamide, N1-[(1S,2R)-3-[[(4-fluorophenyl)sulfonyl](2-methylpropyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



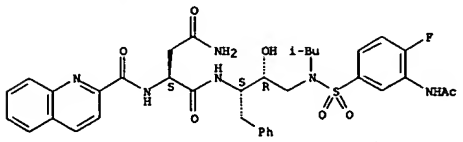
RN 160230-19-3 CAPLUS
CN Butanediamide, N1-[(1S,2R)-3-[[[4-(acetylamino)-3-fluorophenyl]sulfonyl](2-methylpropyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



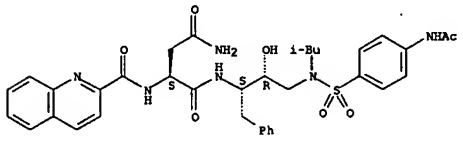
RN 160230-20-6 CAPLUS
CN Butanediamide, N1-[(1S,2R)-3-[[[3-(acetylamino)-4-fluorophenyl]sulfonyl](2-methylpropyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



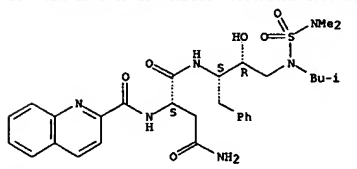
RN 160230-21-7 CAPLUS
CN Butanediamide, N1-[(1S,2R)-3-[[[4-(acetylamino)phenyl]sulfonyl](2-methylpropyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



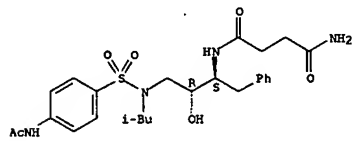
RN 160230-22-8 CAPLUS
CN Butanediamide, N1-[(1S,2R)-3-[[[2-(acetylamino)-4-methyl-5-thiazolyl]sulfonyl](2-methylpropyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



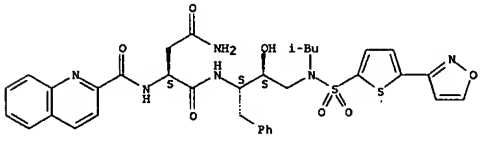
RN 160230-50-2 CAPLUS
CN Butanediamide, N-[(1S,2R)-3-[[[4-(acetylamino)phenyl]sulfonyl](2-methylpropyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



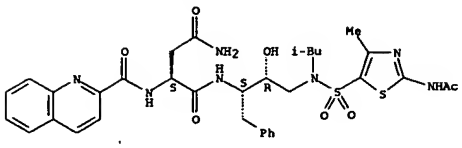
RN 160231-93-6 CAPLUS
CN Butanediamide, N1-[(1S,2S)-2-hydroxy-3-[[[5-(3-isoxazolyl)-2-thienyl]sulfonyl](2-methylpropyl)amino]-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



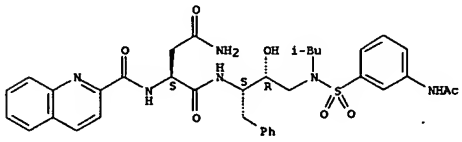
RN 160231-96-9 CAPLUS
CN Butanediamide, N1-[(1S,2R)-3-[[[4-(acetylamino)-3-fluorophenyl]sulfonyl](phenylmethyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



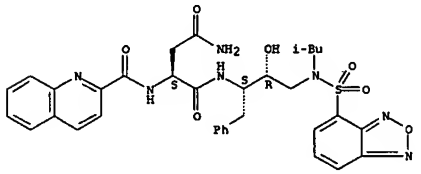
RN 160230-23-9 CAPLUS
CN Butanediamide, N1-[(1S,2R)-3-[[[3-(acetylamino)phenyl]sulfonyl](2-methylpropyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



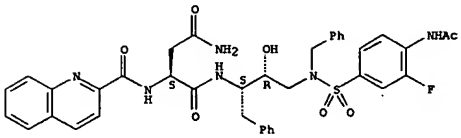
RN 160230-24-0 CAPLUS
CN Butanediamide, N1-[(1S,2R)-3-[(2,1,3-benzoxadiazol-4-ylsulfonyl)(2-methylpropyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



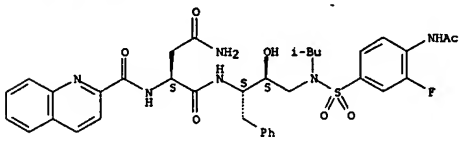
RN 160230-25-1 CAPLUS
CN Butanediamide, N1-[(1S,2R)-3-[[(dimethylamino)sulfonyl](2-methylpropyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



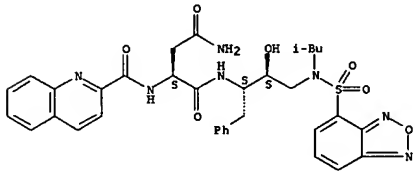
RN 160333-42-6 CAPLUS
CN Butanediamide, N1-[(1S,2S)-3-[[[4-(acetylamino)-3-fluorophenyl]sulfonyl](2-methylpropyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 160333-43-7 CAPLUS
CN Butanediamide, N1-[(1S,2S)-3-[(2,1,3-benzoxadiazol-4-ylsulfonyl)(2-methylpropyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

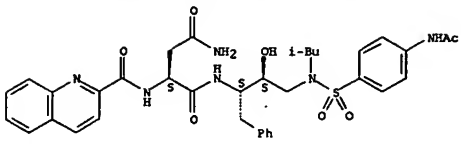
Absolute stereochemistry.



RN 160333-44-8 CAPLUS
CN Butanediamide, N1-[(1S,2S)-3-[[[4-(acetylamino)phenyl]sulfonyl](2-methylpropyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

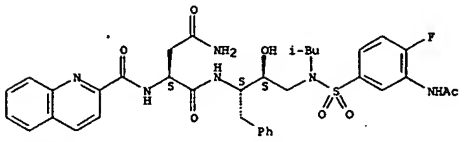
Absolute stereochemistry.

L4 ANSWER 9 OF 23 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



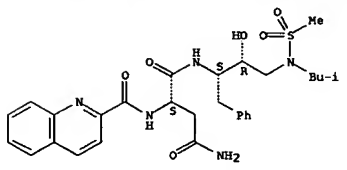
RN 160333-45-9 CAPLUS
CN Butanediamide, N1-[(1S,2S)-3-[[[3-(acetylamino)-4-fluorophenyl]sulfonyl](2-methylpropyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 77 THERE ARE 77 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 10 OF 23 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



L4 ANSWER 10 OF 23 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1998:501276 CAPLUS
DOCUMENT NUMBER: 129:170511
TITLE: Use of quinoxalines in three-way combinations with protease inhibitors and reverse transcriptase inhibitors as a drug for treating AIDS and/or HIV infections
INVENTOR(S): Paessens, Arnold; Blunck, Martin; Riess, Guenter; Kleim, Joerg-Peter; Roesner, Manfred
PATENT ASSIGNEE(S): Bayer A.-G., Germany
SOURCE: Ger. Offen., 22 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19703131	A1	19980730	DE 1997-19703131	19970129
CA 2278773	AA	19980730	CA 1998-2278773	19980115
WO 9832442	A1	19980730	WO 1998-EP197	19980115
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9860940	A1	19980818	AU 1998-60940	19980115
EP 977570	A1	20000209	EP 1998-905297	19980115
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI				
BR 9807523	A	20000321	BR 1998-7523	19980115
JP 2001511124	T2	20010807	JP 1998-531540	19980115
ZA 9800679	A	19980805	ZA 1998-679	19980128
NO 9903670	A	19990910	NO 1999-3670	19990728
MX 9907077	A	20000531	MX 1999-7077	19990729

PRIORITY APPLN. INFO.: DE 1997-19703131 A 19970129
WO 1998-EP197 W 19980115

AB Quinoxaline derivs. in combination with protease inhibitors and reverse transcriptase inhibitors inhibited HIV replication in human lymphocytes. Such 3-way combinations are synergistic and may be used to treat persons with HIV infections or AIDS.

IT 181703-69-5, AM 11686
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(AIDS and HIV infections treatment by combinations of quinoxalines and reverse transcriptase inhibitors with protease inhibitors such as)

RN 181703-69-5 CAPLUS
CN Butanediamide, N1-[(1S,2R)-2-hydroxy-3-[(2-methylpropyl)(methylsulfonyl)amino]-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

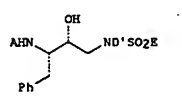
Absolute stereochemistry.

L4 ANSWER 11 OF 23 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1997:9928 CAPLUS
DOCUMENT NUMBER: 126:144117
TITLE: Preparation of sulfonamide inhibitors of aspartyl protease
INVENTOR(S): Tung, Roger D.; Murcko, Mark A.; Bhisetti, Govinda R.
PATENT ASSIGNEE(S): Vertex Pharmaceuticals, Incorporated, USA
SOURCE: U.S., 87 pp., Cont.-in-part of U.S. Ser. No. 941,982, abandoned.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 5
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5585397	A	19961217	US 1993-142327	19931124
WO 9405639	A1	19940317	WO 1993-US8458	19930907
W: AT, AU, BB, BG, BR, BY, CA, CH, CZ, DE, DK, ES, FI, GB, HU, JP, KP, KR, KZ, LK, LU, LV, MG, MN, MW, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SK, UA, US, UZ, VN				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
EP 885887	A2	19981223	EP 1998-113921	19930907
EP 885887	A3	19990203		
EP 885887	B1	20030528		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE				
US 5783701	A	19980721	US 1995-393460	19950223
US 5723490	A	19980303	US 1995-424819	19950419
US 5856353	A	19990105	US 1995-477937	19950607
US 6372778	B1	20020416	US 1995-484326	19950607
US 5977137	A	19991102	US 1998-115394	19980714
US 6004957	A	19991221	US 1998-121008	19980722
US 6392046	B1	20020521	US 1999-409808	19990930
US 2003064977	A1	20030403	US 2002-94763	20020308
US 6720335	B2	20040413		
US 2003069222	A1	20030410	US 2002-94790	20020308
US 2004167116	A1	20040826	US 2004-786997	20040224

PRIORITY APPLN. INFO.: US 1992-941982 B2 19920908
WO 1993-US8458 W 19930907
EP 1993-921428 A3 19930907
US 1993-142327 A2 19931124
US 1995-393460 B2 19950223
US 1995-484326 A3 19950607
US 1998-115394 A3 19980714
US 1999-409808 A3 19990930
US 2002-94763 A1 20020308

OTHER SOURCE(S): MARPAT 126:144117
GI



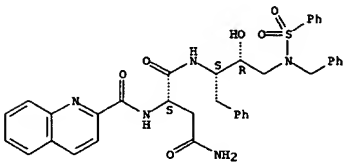
I

AB The title compds. I [A = 3-tetrahydrofuryloxycarbonyl; D' = (un)substituted alkyl; E = (un)substituted aryl] are prepared This invention also relates to pharmaceutical compns. comprising these compds. The compds. and pharmaceutical compns. of this invention are particularly well suited for inhibiting HIV-1 and HIV-2 protease activity and consequently, may be advantageously used as antiviral agents against the HIV-1 and HIV-2 viruses. This invention also relates to methods for inhibiting the activity of HIV aspartyl protease using the compds. of this invention and methods for screening compds. for anti-HIV activity. The title compds. inhibit HIV replication at concentration of ≤ 100 nM.

IT **160230-05-7P 160230-06-8P 160230-07-9P**
160230-08-0P 160230-09-1P 160230-10-4P
160230-11-5P 160230-12-6P 160230-13-7P
160230-14-8P 160230-15-9P 160230-16-0P
160230-17-1P 160230-18-2P 160230-19-3P
160230-20-6P 160230-21-7P 160230-22-8P
160230-23-9P 160230-24-0P 160230-25-1P
160230-50-2P 160231-93-6P 160231-96-9P
160333-42-6P 160333-43-7P 160333-44-8P
160333-45-9P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of sulfonamide inhibitors of aspartyl protease)

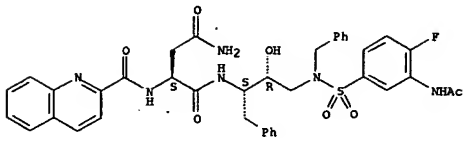
RN 160230-05-7 CAPLUS
CN Butanediamide, N1-[(1S,2R)-2-hydroxy-1-(phenylmethyl)-3-[(phenylmethyl)(phenylsulfonyl)amino]propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



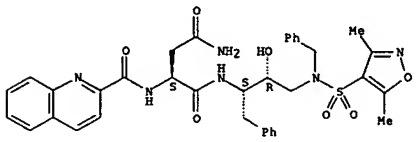
RN 160230-06-8 CAPLUS
CN Butanediamide, N1-[(1S,2R)-3-[[[3-(acetylamino)-4-fluorophenyl]sulfonyl](phenylmethyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



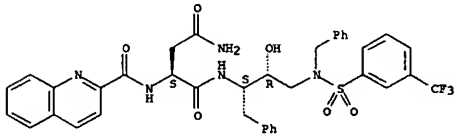
RN 160230-07-9 CAPLUS
CN Butanediamide, N1-[(1S,2R)-3-[[(3,5-dimethyl-4-isoxazolyl)sulfonyl](phenylmethyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



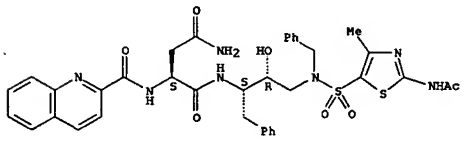
RN 160230-08-0 CAPLUS
CN Butanediamide, N1-[(1S,2R)-2-hydroxy-1-(phenylmethyl)-3-[(phenylmethyl)[[3-(trifluoromethyl)phenyl]sulfonyl]amino]propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



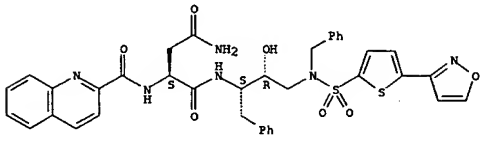
RN 160230-09-1 CAPLUS
CN Butanediamide, N1-[(1S,2R)-3-[[[2-(acetylamino)-4-methyl-5-thiazolyl]sulfonyl](phenylmethyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



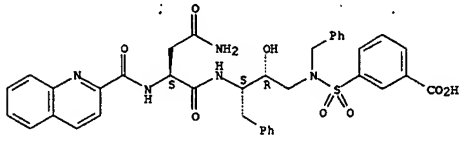
RN 160230-10-4 CAPLUS
CN Butanediamide, N1-[(1S,2R)-2-hydroxy-3-[[[5-(3-isoxazolyl)-2-thienyl]sulfonyl](phenylmethyl)amino]-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



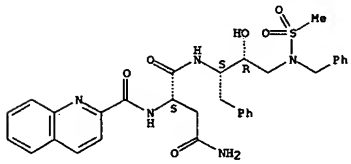
RN 160230-11-5 CAPLUS
CN Benzoic acid, 3-[[[(2R,3S)-3-[[(2S)-4-amino-1,4-dioxo-2-[(2-quinolinylcarbonyl)amino]butyl]amino]-2-hydroxy-4-phenylbutyl](phenylmethyl)amino]sulfonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



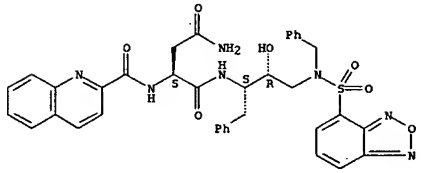
RN 160230-12-6 CAPLUS
CN Butanediamide, N1-[(1S,2R)-2-hydroxy-3-[(methylsulfonyl)(phenylmethyl)amino]-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



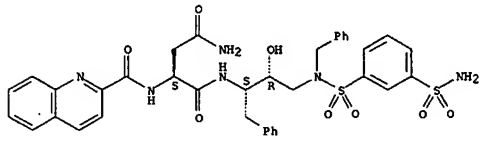
RN 160230-13-7 CAPLUS
CN Butanediamide, N1-[(1S,2R)-3-[(2,1,3-benzoxadiazol-4-ylsulfonyl)(phenylmethyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



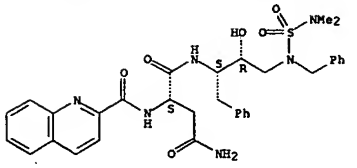
RN 160230-14-8 CAPLUS
CN Butanediamide, N1-[(1S,2R)-3-[[[3-(aminosulfonyl)phenyl]sulfonyl](phenylmethyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



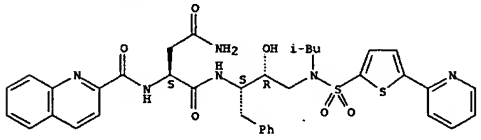
RN 160230-15-9 CAPLUS
CN Butanediamide, N1-[(1S,2R)-3-[[(dimethylamino)sulfonyl](phenylmethyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



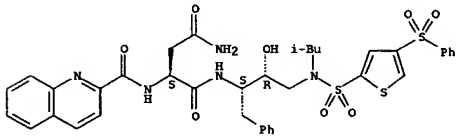
RN 160230-16-0 CAPLUS
CN Butanediamide, N1-[(1S,2R)-2-hydroxy-3-[(2-methylpropyl)[[5-(2-pyridinyl)-2-thienyl]sulfonyl]amino]-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



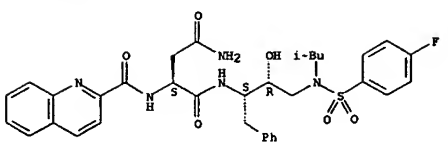
RN 160230-17-1 CAPLUS
CN Butanediamide, N1-[(1S,2R)-2-hydroxy-3-[(2-methylpropyl)[[4-(phenylsulfonyl)-2-thienyl]sulfonyl]amino]-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



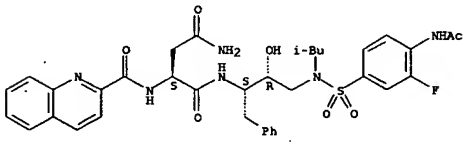
RN 160230-18-2 CAPLUS
CN Butanediamide, N1-[(1S,2R)-3-[[(4-fluorophenyl)sulfonyl](2-methylpropyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



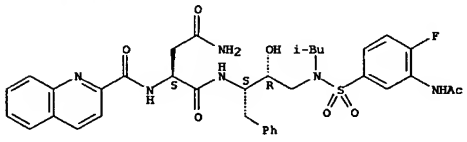
RN 160230-19-3 CAPLUS
CN Butanediamide, N1-[(1S,2R)-3-[[[4-(acetylamino)-3-fluorophenyl]sulfonyl](2-methylpropyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



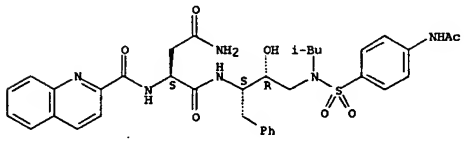
RN 160230-20-6 CAPLUS
CN Butanediamide, N1-[(1S,2R)-3-[[[3-(acetylamino)-4-fluorophenyl]sulfonyl](2-methylpropyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



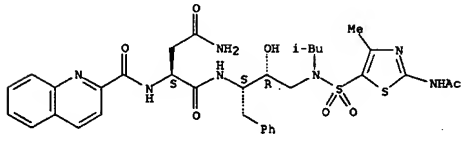
RN 160230-21-7 CAPLUS
CN Butanediamide, N1-[(1S,2R)-3-[[[4-(acetylamino)phenyl]sulfonyl](2-methylpropyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



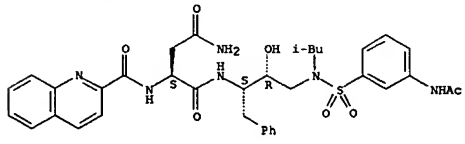
RN 160230-22-8 CAPLUS
CN Butanediamide, N1-[(1S,2R)-3-[[[2-(acetylamino)-4-methyl-5-thiazolyl]sulfonyl](2-methylpropyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



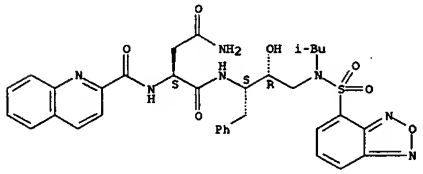
RN 160230-23-9 CAPLUS
CN Butanediamide, N1-[(1S,2R)-3-[[[3-(acetylamino)phenyl]sulfonyl](2-methylpropyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



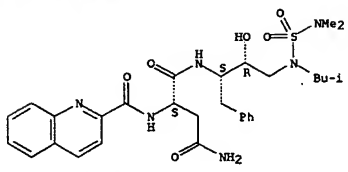
RN 160230-24-0 CAPLUS
CN Butanediamide, N1-[(1S,2R)-3-[(2,1,3-benzoxadiazol-4-ylsulfonyl)(2-methylpropyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



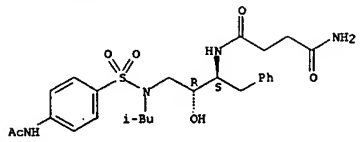
RN 160230-25-1 CAPLUS
CN Butanediamide, N1-[(1S,2R)-3-[[(dimethylamino)sulfonyl](2-methylpropyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



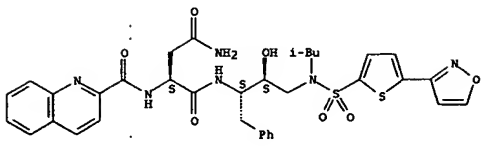
RN 160230-50-2 CAPLUS
CN Butanediamide, N-[(1S,2R)-3-[[[4-(acetylamino)phenyl]sulfonyl](2-methylpropyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



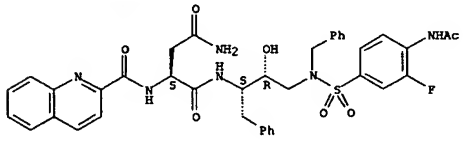
RN 160231-93-6 CAPLUS
CN Butanediamide, N1-[(1S,2S)-2-hydroxy-3-[[[5-(3-isoxazolyl)-2-thienyl]sulfonyl](2-methylpropyl)amino]-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



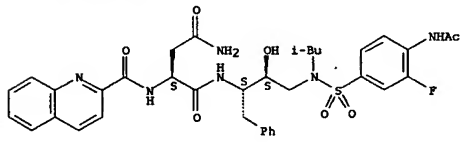
RN 160231-96-9 CAPLUS
CN Butanediamide, N1-{(1S,2R)-3-[[[4-(acetylamino)-3-fluorophenyl]sulfonyl](phenylmethyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



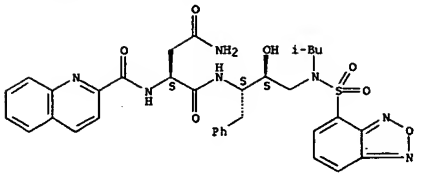
RN 160333-42-6 CAPLUS
CN Butanediamide, N1-[(1S,2S)-3-[[[4-(acetylamino)-3-fluorophenyl]sulfonyl](2-methylpropyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



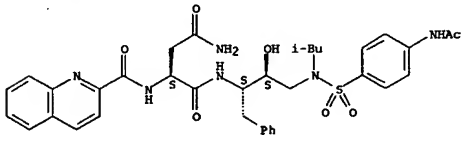
RN 160333-43-7 CAPLUS
CN Butanediamide, N1-[(1S,2S)-3-[(2,1,3-benzoxadiazol-4-ylsulfonyl)(2-methylpropyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



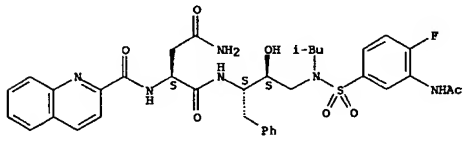
RN 160333-44-8 CAPLUS
CN Butanediamide, N1-[(1S,2S)-3-[[[4-(acetylamino)phenyl]sulfonyl](2-methylpropyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 160333-45-9 CAPLUS
CN Butanediamide, N1-[(1S,2S)-3-[[[3-(acetylamino)-4-fluorophenyl]sulfonyl](2-methylpropyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



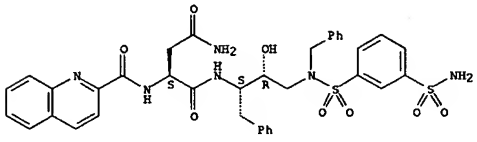
IT **186463-21-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of sulfonamide inhibitors of aspartyl protease)
RN 186463-21-8 CAPLUS
CN Butanediamide, N1-[(1S,2R)-3-[[[3-(aminosulfonyl)phenyl]sulfonyl](phenylmethyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-

quinolinylcarbonyl)amino]-, (2S)-, mono(trifluoroacetate) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 160230-14-8
CMF C37 H38 N6 O8 S2

Absolute stereochemistry.



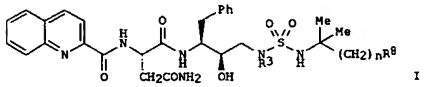
CM 2

CRN 76-05-1
CMF C2 H F3 O2

ACCESSION NUMBER: 1996:725344 CAPLUS
DOCUMENT NUMBER: 126:75247
TITLE: Preparation of α- and β-amino acid hydroxyethylamino sulfonyl urea derivatives as retroviral protease inhibitors
INVENTOR(S): Vazquez, Michael L.; Mueller, Richard A.; Talley, John J.; Getman, Daniel P.; Decrescenzo, Gary A.; Sun, Eric T.
PATENT ASSIGNEE(S): G.D. Searle and Co., USA
SOURCE: U.S., 37 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5578606	A	19961126	US 1992-968712	19921030
US 6022872	A	20000208	US 1996-709069	19960906
US 6211176	B1	20010403	US 1999-345739	19990701
US 6403585	B1	20020611	US 2000-731911	20001208
US 2003144342	A1	20030731	US 2002-138534	20020506
US 6683648	B2	20040127		
US 2004171653	A1	20040902	US 2003-689513	20031021
PRIORITY APPLN. INFO.:			US 1992-968712	A3 19921030
			US 1996-709069	A1 19960906
			US 1999-345739	A1 19990701
			US 2000-731911	A1 20001208
			US 2002-138534	A1 20020506

OTHER SOURCE(S): MARPAT 126:75247
GI



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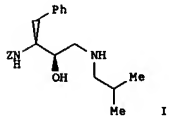

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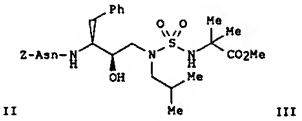


III

AB α- And β-amino acid hydroxyethylamino sulfonyl urea derivative compds., e.g. I [R3 = C1-8 alkyl, (un)substituted C1-8 alkylphenyl, C1-8 heteroaralkyl; R8 = (un)substituted Ph, heterocyclyl, CN, OH, CO2H, C1-8 alkylthio, (un)substituted phenylsulfonyl, C1-8 alkanoyl, C1-8 alkoxycarbonyl, C1-8 dialkylaminocarbonyl, N-C1-8- alkyl-N-phenylcarbamoyl, 2-heterocyclylethoxy, heterocyclyl; n = 0-2], are

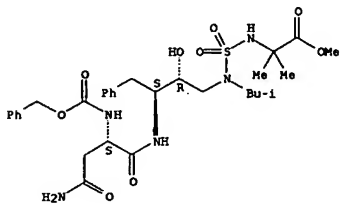
L4 ANSWER 12 OF 23 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
effective as retroviral protease inhibitors, and in particular as inhibitors of HIV protease. Thus, coupling of protected amino(hydroxy)phenylbutylamine II (Z = PhCH2O2C) (prepd. in 3 steps from chloromethyl ketone Z-L-Phe-CH2Cl) with ClSO2NHCMe2CO2Me, followed by hydrogenolysis and coupling with 2-Asn-OH gave inhibitor III.

IT **185256-67-1P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of hydroxyethylamino sulfonyl urea peptide derivs. as retroviral protease inhibitors)

RN 185256-67-1 CAPLUS

CN 10-Thia-2,5,9,11-tetraazatridecanedioic acid, 3-(2-amino-2-oxoethyl)-7-hydroxy-12,12-dimethyl-9-(2-methylpropyl)-4-oxo-6-(phenylmethyl)-, 13-methyl 1-(phenylmethyl) ester, 10,10-dioxide, [3S-(3R*,6R*,7S*)]- (9CI) (CA INDEX NAME)

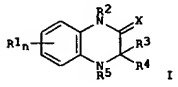
Absolute stereochemistry.



L4 ANSWER 13 OF 23 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1996:601709 CAPLUS
DOCUMENT NUMBER: 125:238651
TITLE: Use of quinoxalines and protease inhibitors in a composition for the treatment of AIDS and/or HIV infections
INVENTOR(S): Paessens, Arnold; Blunck, Martin; Riess, Guenther; Klein, Joerg-Peter; Roesner, Manfred
PATENT ASSIGNEE(S): Bayer A.-G., Germany
SOURCE: Eur. Pat. Appl., 24 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 728481	A2	19960828	EP 1996-102129	19960214
EP 728481	A3	19980708		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
DE 19506742	A1	19960829	DE 1995-19506742	19950227
AU 9645615	A1	19960905	AU 1996-45615	19960220
AU 710158	B2	19990916		
CA 2170222	AA	19960828	CA 1996-2170222	19960223
FI 9600850	A	19960828	FI 1996-850	19960223
JP 08245392	A2	19960924	JP 1996-60286	19960223
IL 117247	A1	20001031	IL 1996-117247	19960223
NO 9600775	A	19960828	NO 1996-775	19960226
ZA 9601516	A	19960903	ZA 1996-1516	19960226
BR 9600809	A	19971223	BR 1996-809	19960226
CN 1141196	A	19970129	CN 1996-102709	19960227
PRIORITY APPLN. INFO.:			DE 1995-19506742 A	19950227
OTHER SOURCE(S):	MARPAT 125:238651			

GI



I

AB Combinations of a quinoxaline derivative [I; R1 = halo, OH, NO2, (substituted) amino, N3, CF3, CF3O, C1-8 alkyl, CN, (substituted) Ph, N-heterocyclyl, etc.; R2, R5 = H, OH, C1-6 alkoxy, aryloxy, C1-6 acyloxy, CN, (substituted) amino, (substituted) C1-8 alkyl, (substituted) C2-8 alkenyl, (substituted) C3-8 alkynyl, (substituted) C3-8 cycloalk(en)yl, etc.; R3, R4 = H, (substituted) C1-8 alkyl, (substituted) C2-8 alkenyl, (substituted) C3-8 cycloalk(en)yl, (substituted)aryl, etc.; or R3R4 or R3R5 complete a (substituted) ring; X = O, S, Se, NR2; n = 0-4] and a peptidomimetic protease inhibitor are useful for treatment of HIV infections and AIDS. Thus, I [R1 = 6-MeO, R2 = R3 = H, R4 = (S)-MeSCH2, R5 = i-PrO2C, X = S] (0.7-6 nM) and saquinavir (6-50 nM) synergistically inhibited syncytium formation in HIV-infected human lymphocytes in vitro.

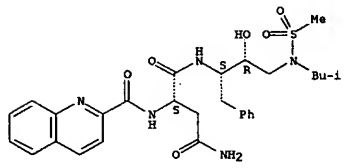
L4 ANSWER 13 OF 23 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

IT **181703-69-5**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(use of quinoxalines and protease inhibitors for treatment of AIDS and HIV infections)

RN 181703-69-5 CAPLUS

CN Butanediamide, N1-{(1S,2R)-2-hydroxy-3-[(2-methylpropyl)(methylsulfonyl)amino]-1-(phenylmethyl)propyl}-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 14 OF 23 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1996:153437 CAPLUS
DOCUMENT NUMBER: 124:220480
TITLE: Retroviral protease inhibitor combinations
INVENTOR(S): Bryant, Martin L.; Potts, Karen E.; Smidt, Mary; Tucker, Simon P.
PATENT ASSIGNEE(S): G.D. Searle and Co., USA
SOURCE: PCT Int. Appl., 64 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9533464	A2	19951214	WO 1995-US6673	19950602
WO 9533464	A3	19960104		
W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD, MG, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TT				
RW: KE, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
CA 2191948	AA	19951214	CA 1995-2191948	19950602
AU 9526510	A1	19960104	AU 1995-26510	19950602
AU 696299	B2	19980903		
EP 762880	A1	19970319	EP 1995-921428	19950602
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
BR 9507912	A	19970812	BR 1995-7912	19950602
CN 1166786	A	19971203	CN 1995-194464	19950602
HU 76979	A2	19980128	HU 1996-3328	19950602
JP 10505324	T2	19980526	JP 1995-501057	19950602
NZ 287702	A	20000623	NZ 1995-287702	19950602
US 6100277	A	20000808	US 1995-458154	19950602
PL 180070	B1	20001229	PL 1995-317425	19950602
RU 2166317	C2	20010510	RU 1997-100123	19950602
NO 9605136	A	19970120	NO 1996-5136	19961202
FI 9604835	A	19970129	FI 1996-4835	19961203
US 2003207813	A1	20031106	US 2002-253899	20020925
PRIORITY APPLN. INFO.:			US 1994-253638 A2	19940603
			WO 1995-US6673 W	19950602
			US 1996-737960 B1	19961209

AB A method is disclosed for the treatment of mammalian retrovirus infections, e.g. HIV, using combinations of retroviral protease inhibitors which are effective in preventing the replication of the retroviruses in vitro or in vivo. In particular, the invention provides protease inhibitor compds. used in combination therapy with other protease inhibitor compds. Also disclosed is combination therapy with a combination of protease inhibitors and antiviral agents other than protease inhibitors. Preparation and activity of selected inhibitors is included.

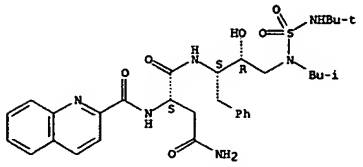
IT **160676-92-6**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(retroviral protease inhibitor combinations, and protease inhibitor preparation)

RN 160676-92-6 CAPLUS

CN Butanediamide, N1-[3-[[[(1,1-dimethylethyl)amino]sulfonyl](2-methylpropyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-

L4 ANSWER 14 OF 23 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
quinolinylcarbonyl)amino]-, [1S-[1R*(R*),2S*]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 15 OF 23 CAPLUS COPYRIGHT 2005 ACS on STN

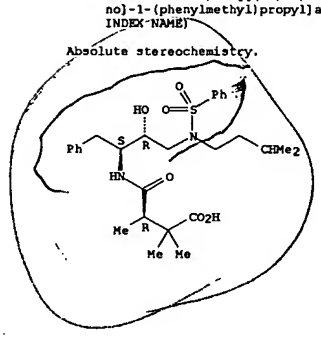
ACCESSION NUMBER: 1996:47171 CAPLUS
DOCUMENT NUMBER: 124:193129
TITLE: Determination of protein binding by in vitro charcoal adsorption
AUTHOR(S): Yuan, Jinhua; Yang, Dai Chang; Birkmeier, Jill; Stolzenbach, James
CORPORATE SOURCE: Pharmacokinetics, Bioanalytical and Radiochemistry Function, G. D. Searle Research and Development, Skokie, IL, 60077, USA
SOURCE: Journal of Pharmacokinetics and Biopharmaceutics (1995), 23(1), 41-55
CODEN: JPBPBJ; ISSN: 0090-466X
PUBLISHER: Plenum
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Certain compds. such as SC-52151 have extensive nonspecific adsorption to the ultrafiltration devices or to dialysis membranes and therefore can not be measured by the conventional ultrafiltration or equilibrium dialysis methods. A new method based on charcoal adsorption was developed to overcome this difficulty. Unlike many conventional methods, which are based on the separation of free drug from bound drug under equilibrium conditions, the new method is operated under nonequil. conditions and involves measuring the time course of decline of the percentage of bound drug remaining in plasma while the free drug is being removed by charcoal adsorption. Theor. aspects of the method and the data processing procedure are presented. SC-98A, a compound with minimal nonspecific adsorption to the ultrafiltration membrane, was used to demonstrate the applicability of this method against the ultrafiltration method. Using this method, the protein binding of SC-52151 in human plasma at 1.0 μg/mL was determined to be in the range of 91.4-97.7% at room temperature

IT 157445-98-2, SC 98A
RL: BPR (Biological process); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); PROC (Process); USES (Uses)
(protein binding determination by in vitro charcoal adsorption)

RN 157445-98-2 CAPLUS
CN Butanoic acid, 4-[[(1S,2R)-2-hydroxy-3-[(3-methylbutyl)(phenylsulfonyl)amino]-1-(phenylmethyl)propyl]amino]-2,2,3-trimethyl-4-oxo-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 16 OF 23 CAPLUS COPYRIGHT 2005 ACS on STN

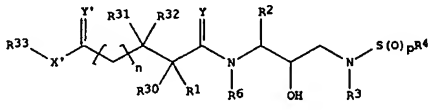
ACCESSION NUMBER: 1995:964989 CAPLUS
DOCUMENT NUMBER: 124:176937
TITLE: N-[(Succinoylamino)hydroxypropyl]sulfonamides useful as retroviral protease inhibitors
INVENTOR(S): Vazquez, Michael L.; Mueller, Richard A.; Talley, John J.; Getman, Daniel; Decrescenzo, Gary A.; Freskos, John N.
PATENT ASSIGNEE(S): G. D. Searle and Co., USA
SOURCE: U.S., 32 pp. Cont.-in-part of U.S. Ser. No. 935,490, abandoned
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5463104	A	19951031	US 1993-110912	19930824
AT 154800	E	19970715	AT 1993-920213	19930824
ES 2103488	T3	19970916	ES 1993-920213	19930824
US 5714605	A	19980203	US 1995-541350	19951010
US 5760076	A	19980602	US 1995-541747	19951010
US 6022994	A	20000208	US 1998-41016	19980312
US 6313345	B1	20011106	US 1999-419816	19991018
US 2002137942	A1	20020926	US 2001-884462	20010620
US 6469207	B2	20021022		
US 2003220508	A1	20031127	US 2002-237184	20020909
US 6727282	B2	20040427		
US 2005004043	A1	20050106	US 2004-784916	20040224

PRIORITY APPLN. INFO.: US 1992-935490 B2 19920825
US 1993-110912 A3 19930824
US 1995-541350 A1 19951010
US 1995-541747 A1 19951010
US 1998-41016 A1 19980312
US 1999-419816 A1 19991018
US 2001-884462 A1 20010620
US 2002-237184 A1 20020909

OTHER SOURCE(S): MARPAT 124:176937
GI

L4 ANSWER 16 OF 23 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



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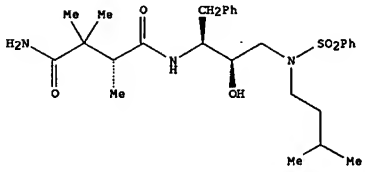


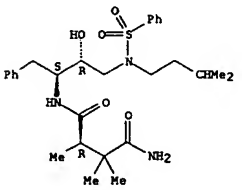
II

AB Succinoylamino hydroxyethylamino sulfonamide compds. I or a pharmaceutically acceptable salt or ester thereof, wherein p represents 0, 1 or 2; n represents either 0 or 1; X' represents N(R34) or O; or R33X' represents cycloalkyl or aryl radicals; Y and Y' each independently represent O or S; R1, R3G, R31 and R32 each independently represent hydrogen, OH, (CH2)C(O)CH3, CH2SO2NH2, CO2CH3, CONHCH3, CON(CH3)2, CH2C(O)NHCH3, CH2C(O)N(CH3)2, CONH2, C(CH3)2(SH), C(CH3)2(SCH3), C(CH3)2[S(O)CH3), C(CH3)2[S(O)2CH3), alkyl, haloalkyl, alkenyl, alkynyl, aralkyl or cycloalkyl radicals, or the side chain of the amino acid asparagine, S-Me cysteine or the corresponding sulfoxide or sulfone derivs. thereof, leucine, isoleucine, allo-isoleucine, tert-leucine, phenylalanine, ornithine, alanine, norleucine, glutamine, valine, threonine, serine, o-alkyl serine, aspartic acid, β-cyanoalanine or allothreonine; or R30 and R32 together with the carbon atoms to which they are attached form a cycloalkyl radical; R2 = e.g., alkyl, aryl, cycloalkyl; R3, R33, R34 = e.g., H, alkyl, haloalkyl; R4 = e.g., alkyl, haloalkyl, alkenyl; R6 = H, alkyl; are effective as retroviral protease inhibitors, and in particular as inhibitors of HIV protease. Thus, e.g., butanediamide II was prepared by coupling of benzyl (R)-2,2,3-trimethylsuccinate (preparation given) with 2(R)-hydroxy-3-[(3-methylbutyl)(phenylsulfonyl)amino]-1(S)-(phenylmethyl)propylamine (preparation given) followed by benzyl ester hydrogenolysis and amidation, and exhibited IC50 = 2 nM for inhibition of HIV protease.

IT 157445-96-0P 157445-97-1P 157445-98-2P
157445-99-3P 157446-00-9P 157446-02-1P
157446-03-2P 157446-04-3P 157446-05-4P
157446-06-5P 157446-07-6P 157446-08-7P
157446-09-8P 157474-44-7P 173590-71-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(N-[(succinoylamino)hydroxypropyl]sulfonamides useful as retroviral protease inhibitors)

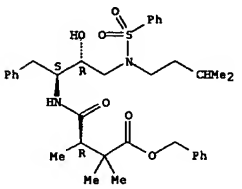
L4 ANSWER 16 OF 23 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
RN 157445-96-0 CAPLUS
CN Butanediamide, N4-[(1S,2R)-2-hydroxy-3-[(3-methylbutyl)(phenylsulfonyl)amino]-1-(phenylmethyl)propyl]-2,2,3-trimethyl-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 157445-97-1 CAPLUS
CN Butanoic acid, 4-[[2-hydroxy-3-[(3-methylbutyl)(phenylsulfonyl)amino]-1-(phenylmethyl)propyl]amino]-2,2,3-trimethyl-4-oxo-, phenylmethyl ester, [1S-[1R*(S*),2S*]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

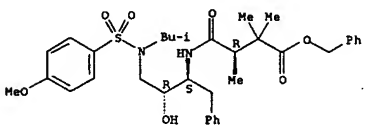


RN 157445-98-2 CAPLUS
CN Butanoic acid, 4-[[(1S,2R)-2-hydroxy-3-[(3-methylbutyl)(phenylsulfonyl)amino]-1-(phenylmethyl)propyl]amino]-2,2,3-trimethyl-4-oxo-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

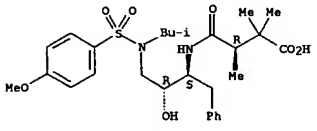
L4 ANSWER 16 OF 23 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
methylpropyl)amino]-1-(phenylmethyl)propyl]amino]-2,2,3-trimethyl-4-oxo-, phenylmethyl ester, [1S-[1R*(S*),2S*]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



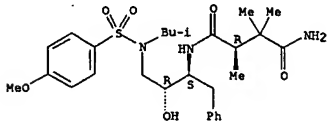
RN 157446-03-2 CAPLUS
CN Butanoic acid, 4-[[2-hydroxy-3-[[(4-methoxyphenyl)sulfonyl](2-methylpropyl)amino]-1-(phenylmethyl)propyl]amino]-2,2,3-trimethyl-4-oxo-, [1S-[1R*(S*),2S*]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 157446-04-3 CAPLUS
CN Butanediamide, N4-[(1S,2R)-2-hydroxy-3-[[(4-methoxyphenyl)sulfonyl](2-methylpropyl)amino]-1-(phenylmethyl)propyl]-2,2,3-trimethyl-, (3R)- (9CI) (CA INDEX NAME)

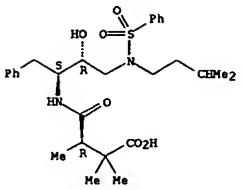
Absolute stereochemistry.



RN 157446-05-4 CAPLUS
CN Butanediamide, N4-[(1S,2R)-2-hydroxy-3-[[(4-methoxyphenyl)sulfonyl](3-methylbutyl)amino]-1-(phenylmethyl)propyl]-2,2,3-trimethyl-, (3R)- (9CI) (CA INDEX NAME)

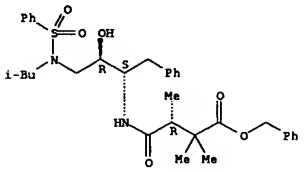
Absolute stereochemistry.

L4 ANSWER 16 OF 23 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



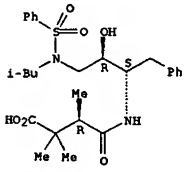
RN 157445-99-3 CAPLUS
CN Butanoic acid, 4-[[2-hydroxy-3-[(2-methylpropyl)(phenylsulfonyl)amino]-1-(phenylmethyl)propyl]amino]-2,2,3-trimethyl-4-oxo-, phenylmethyl ester, [1S-[1R*(S*),2S*]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



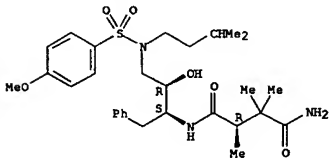
RN 157446-00-9 CAPLUS
CN Butanoic acid, 4-[[2-hydroxy-3-[(2-methylpropyl)(phenylsulfonyl)amino]-1-(phenylmethyl)propyl]amino]-2,2,3-trimethyl-4-oxo-, [1S-[1R*(S*),2S*]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



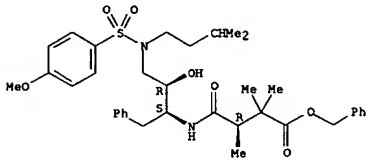
RN 157446-02-1 CAPLUS
CN Butanoic acid, 4-[[2-hydroxy-3-[[(4-methoxyphenyl)sulfonyl](2-

L4 ANSWER 16 OF 23 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



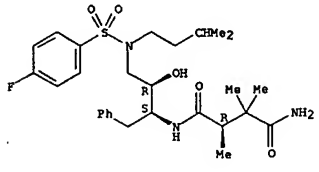
RN 157446-06-5 CAPLUS
CN Butanoic acid, 4-[[2-hydroxy-3-[[(4-methoxyphenyl)sulfonyl](3-methylbutyl)amino]-1-(phenylmethyl)propyl]amino]-2,2,3-trimethyl-4-oxo-, phenylmethyl ester, [1S-[1R*(S*),2S*]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



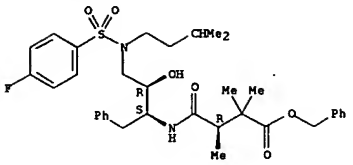
RN 157446-07-6 CAPLUS
CN Butanediamide, N4-[(1S,2R)-3-[[(4-fluorophenyl)sulfonyl](3-methylbutyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-2,2,3-trimethyl-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



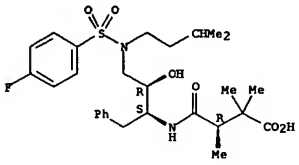
RN 157446-08-7 CAPLUS
CN Butanoic acid, 4-[[3-[[(4-fluorophenyl)sulfonyl](3-methylbutyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]amino]-2,2,3-trimethyl-4-oxo-, phenylmethyl ester, [1S-[1R*(S*),2S*]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



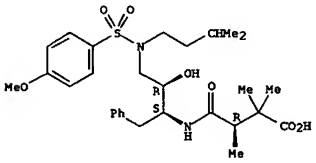
RN 157446-09-8 CAPLUS
CN Butanoic acid, 4-[[3-[[(4-fluorophenyl)sulfonyl](3-methylbutyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]amino]-2,2,3-trimethyl-4-oxo-, [1S-[1R*(S*),2S*]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



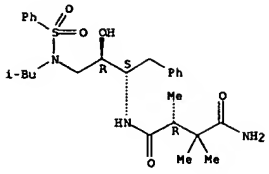
RN 157474-44-7 CAPLUS
CN Butanoic acid, 4-[[2-hydroxy-3-[[(4-methoxyphenyl)sulfonyl](3-methylbutyl)amino]-1-(phenylmethyl)propyl]amino]-2,2,3-trimethyl-4-oxo-, [1S-[1R*(S*),2S*]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 173590-71-1 CAPLUS
CN Butanediamide, N4-[(1S,2R)-2-hydroxy-3-[(2-methylpropyl)(phenylsulfonyl)amino]-1-(phenylmethyl)propyl]-2,2,3-trimethyl-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



ACCESSION NUMBER: 1995:871984 CAPLUS
DOCUMENT NUMBER: 123:279761
TITLE: Hydroxyethylamino sulfonamides useful as retroviral protease inhibitors
INVENTOR(S): Vazquez, Michael L.; Mueller, Richard A.; Talley, John J.; Getman, Daniel P.; Decrescenzo, Gary A.; Freskos, John N.; Bertenshaw, Deborah E.; Heintz, Robert M.
PATENT ASSIGNEE(S): G.D. Searle and Co., USA; Monsanto Co.
SOURCE: PCT Int. Appl., 255 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 6
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9506030	A1	19950302	WO 1994-US9139	19940823
W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, ES, FI, GB, GE, HU, JP, KE, KG, KP, KR, KZ, LK, LT, LU, LV, MD, MG, MN, MW, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SI, SK, TJ, TT, UA, US, US, UZ, VN				
RW: KE, MW, SD, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
US 5843946	A	19981201	US 1993-110911	19930824
US 6060476	A	20000509	US 1994-204827	19940302
AU 9476697	A1	19950321	AU 1994-76697	19940823
EP 715618	A1	19960612	EP 1994-927162	19940823
EP 715618	B1	19981216		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
US 6046190	A	20000404	US 1996-586866	19960124

PRIORITY APPLN. INFO.:
US 1993-110911 A 19930824
US 1994-204827 A 19940302
US 1992-934984 B2 19920825
WO 1993-US7814 A2 19930824
US 1994-204872 B2 19940302
WO 1994-US9139 W 19940823

OTHER SOURCE(S): MARPAT 123:279761

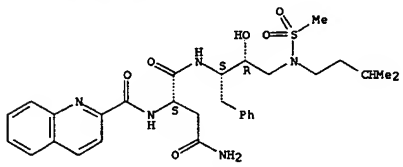
AB Hyroxethylamino sulfonamide compds. AC(:Y)NR6CHR2CHOHCH2NR3S(:O)xR4 [I; R2=(substituted)alkyl, aryl, cycloalkyl, cycloalkylalkyl, aralkyl; R3=H; R3,R4=R2, alkenyl, alkynyl, heterocycloalkyl, -aryl, -aralkyl, -cycloalkyalkyl; R6=H, alkyl; x=1,2; Y=O, S; A=RO, R; R=alkyl, alkenyl; (hetero)aryl, cycloalkyl, cycloalkylalkyl, aralkyl, NH2, mono- or disubstituted amino, etc.] are effective as retroviral protease inhibitors, and in particular as inhibitors of HIV protease. Many inhibitors were prepared by (1) preparing an N-protected amino epoxide and (2) reacting this with an amine and (3) preparing a sulfonamide by reacting with a sulfonyl chloride or sulfonyl anhydride in the presence of an acid scavenger. The amino function of the sulfonamide was then (4) deprotected and (5) reacted with a carboxylate. In vitro HIV protease assays with these compds. revealed inhibitors with IC50's as low as 1.4 nM, e.g. [1S-[1R*(S*),2S*]]-I (A=p-MeOC6H4CH2OCONHCH2CHMe; Y=O; R6=H; R2=benzyl; R3=3-methylbutyl; x=2; R4=phenyl).

IT **159005-89-7P 159005-91-1P 159005-95-5P**
159006-21-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(hydroxyethylamino sulfonamides useful as retroviral protease

inhibitors)

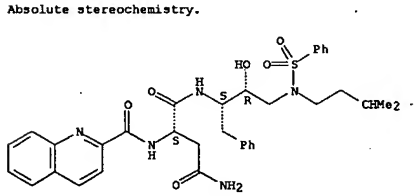
RN 159005-89-7 CAPLUS
CN Butanediamide, N1-[(1S,2R)-2-hydroxy-3-[(3-methylbutyl)(methylsulfonyl)amino]-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



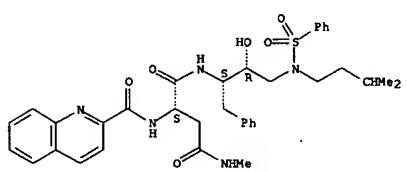
RN 159005-91-1 CAPLUS
CN Butanediamide, N1-[(1S,2R)-2-hydroxy-3-[(3-methylbutyl)(phenylsulfonyl)amino]-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 159005-95-5 CAPLUS
CN Butanediamide, N1-[(1S,2R)-2-hydroxy-3-[(3-methylbutyl)(phenylsulfonyl)amino]-1-(phenylmethyl)propyl]-N4-methyl-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

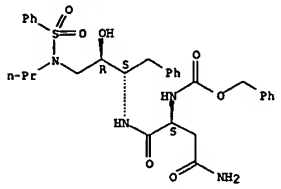
Absolute stereochemistry.



L4 ANSWER 17 OF 23 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

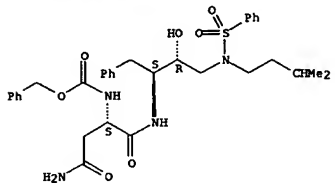
RN 159006-21-0 CAPLUS
CN Carbamic acid, [(1S)-3-amino-1-[[[(1S,2R)-2-hydroxy-1-(phenylmethyl)-3-[(phenylsulfonyl)propylamino]propyl]amino]carbonyl]-3-oxopropyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 159005-92-2 159006-06-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(hydroxyethylamino sulfonamides useful as retroviral protease inhibitors)
RN 159005-92-2 CAPLUS
CN Carbamic acid, [(1S)-3-amino-1-[[[(1S,2R)-2-hydroxy-3-[(3-methylbutyl)(phenylsulfonyl)amino]-1-(phenylmethyl)propyl]amino]carbonyl]-3-oxopropyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

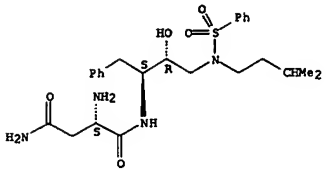
Absolute stereochemistry.



RN 159006-06-1 CAPLUS
CN Butanediamide, 2-amino-N1-[(1S,2R)-2-hydroxy-3-[(3-methylbutyl)(phenylsulfonyl)amino]-1-(phenylmethyl)propyl]-, (2S)- (9CI) (CA INDEX NAME)

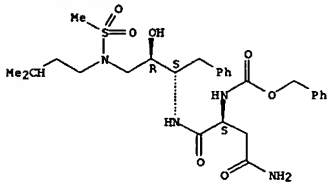
Absolute stereochemistry.

L4 ANSWER 17 OF 23 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



IT 159005-90-0P 159006-05-0P 159006-22-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(hydroxyethylamino sulfonamides useful as retroviral protease inhibitors)
RN 159005-90-0 CAPLUS
CN 2-Thia-3,7,10-triazaundecan-11-oic acid, 9-(2-amino-2-oxoethyl)-5-hydroxy-3-(3-methylbutyl)-8-oxo-6-(phenylmethyl)-, phenylmethyl ester, 2,2-dioxide, (5R,6S,9S)- (9CI) (CA INDEX NAME)

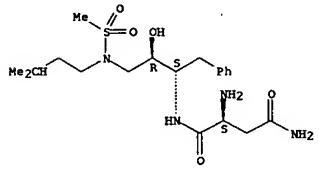
Absolute stereochemistry.



RN 159006-05-0 CAPLUS
CN Butanediamide, 2-amino-N1-[(1S,2R)-2-hydroxy-3-[(3-methylbutyl)(methylsulfonyl)amino]-1-(phenylmethyl)propyl]-, (2S)- (9CI) (CA INDEX NAME)

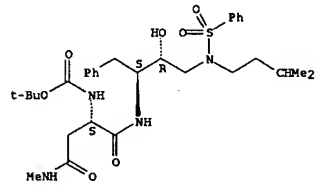
Absolute stereochemistry.

L4 ANSWER 17 OF 23 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



RN 159006-22-1 CAPLUS
CN Carbamic acid, [(1S)-1-[[[(1S,2R)-2-hydroxy-3-[(3-methylbutyl)(phenylsulfonyl)amino]-1-(phenylmethyl)propyl]amino]carbonyl]-3-(methylamino)-3-oxopropyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



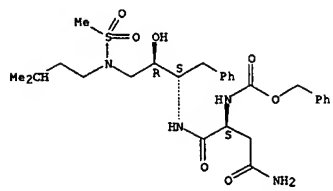
L4 ANSWER 18 OF 23 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1995:352211 CAPLUS
DOCUMENT NUMBER: 122:204547
TITLE: Inhibitors of HIV-1 Protease Containing the Novel and Potent (R)-(Hydroxyethyl)sulfonamide Isostere
AUTHOR(S): Vazquez, Michael L.; Bryant, Martin L.; Clare, Michael; DeCrescenzo, Gary A.; Doherty, Elizabeth M.; Freskos, John N.; Getman, Daniel P.; Houseman, Kathryn A.; Julien, Janet A.; et al.
CORPORATE SOURCE: Searle Discovery Research, Skokie, IL, 60077, USA
SOURCE: Journal of Medicinal Chemistry (1995), 38(4), 581-4
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 122:204547

AB The authors have prepared and tested a series of novel and highly potent HIV-1 protease inhibitors based on the (R)-(hydroxyethyl)sulfonamide isostere. The isotere exhibits enhanced potency relative to the previously reported (hydroxyethyl)urea isotere. The preferred stereochem. for the critical hydroxyl group is R. X-ray crystallog. studies show that these inhibitors bind to the protease in an extended fashion with one of the sulfonamide oxygens forming a hydrogen bond to the key structural water mol. Some of the compds. showed excellent antiviral activity in vitro.

IT 159005-90-0
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(inhibitors of HIV-1 protease containing novel and potent (R)-(hydroxyethyl)sulfonamide isostere in relation to antiviral activity)
RN 159005-90-0 CAPLUS
CN 2-Thia-3,7,10-triazaundecan-11-oic acid, 9-(2-amino-2-oxoethyl)-5-hydroxy-3-(3-methylbutyl)-8-oxo-6-(phenylmethyl)-, phenylmethyl ester, 2,2-dioxide, (5R,6S,9S)- (9CI) (CA INDEX NAME)

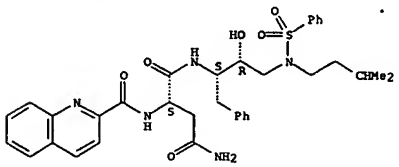
Absolute stereochemistry.



IT 159005-91-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(inhibitors of HIV-1 protease containing novel and potent (R)-(hydroxyethyl)sulfonamide isostere in relation to antiviral activity)
RN 159005-91-1 CAPLUS

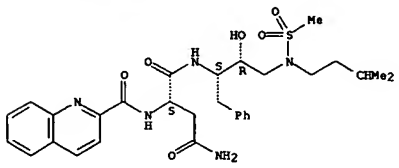
L4 ANSWER 18 OF 23 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
CN Butanediamide, N1-[(1S,2R)-2-hydroxy-3-[(3-methylbutyl)(phenylsulfonyl)amino]-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 159005-89-7P 159005-92-2P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(inhibitors of HIV-1 protease containing novel and potent (R)-(hydroxyethyl)sulfonamide isostere in relation to antiviral activity)
RN 159005-89-7 CAPLUS
CN Butanediamide, N1-[(1S,2R)-2-hydroxy-3-[(3-methylbutyl)(methylsulfonyl)amino]-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

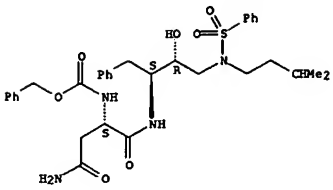
Absolute stereochemistry.



RN 159005-92-2 CAPLUS
CN Carbamic acid, [(1S)-3-amino-1-[[[(1S,2R)-2-hydroxy-3-[(3-methylbutyl)(phenylsulfonyl)amino]-1-(phenylmethyl)propyl]amino]carbonyl]-3-oxopropyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

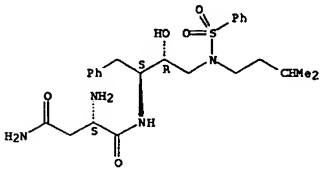
Absolute stereochemistry.

L4 ANSWER 18 OF 23 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



IT 159006-06-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(inhibitors of HIV-1 protease containing novel and potent (R)-(hydroxyethyl)sulfonamide isostere in relation to antiviral activity)
RN 159006-06-1 CAPLUS
CN Butanediamide, 2-amino-N1-[(1S,2R)-2-hydroxy-3-[(3-methylbutyl)(phenylsulfonyl)amino]-1-(phenylmethyl)propyl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

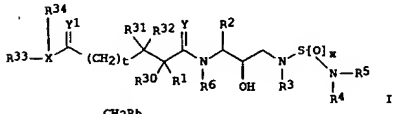


L4 ANSWER 19 OF 23 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1995:340526 CAPLUS
DOCUMENT NUMBER: 122:133838
TITLE: preparation of succinoylamino hydroxyethylamino sulfamic acid derivatives as retroviral protease inhibitors
INVENTOR(S): Vazquez, Michael L.; Mueller, Richard A.; Talley, John J.; Getman, Daniel P.; De Crescenzo, Gary A.; Sun, Eric T.
PATENT ASSIGNEE(S): G.D. Searle and Co., USA; Monsanto Co.
SOURCE: PCT Int. Appl.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

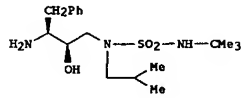
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9410133	A1	19940511	WO 1993-US10460	19931029
W: AT, AU, BB, BG, BR, BY, CA, CH, CZ, DE, DK, ES, FI, GB, HU, JP, KP, KR, KZ, LK, LU, LV, MG, MN, MW, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SK, UA, US, VN				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
CA 2141570	AA	19940511	CA 1993-2141570	19931029
AU 9455892	A1	19940524	AU 1994-55892	19931029
EP 666841	A1	19950816	EP 1994-901230	19931029
EP 666841	B1	19970122		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
AT 148105	E	19970215	AT 1994-901230	19931029
ES 2097023	T3	19970316	ES 1994-901230	19931029
US 5602119	A	19970211	US 1995-379573	19950131
PRIORITY APPLN. INFO.:			US 1992-969683 A	19921030
			WO 1993-US10460 W	19931029

OTHER SOURCE(S): MARPAT 122:133838
GI

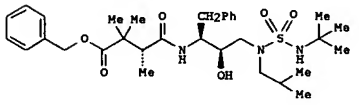
L4 ANSWER 19 OF 23 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



I



II



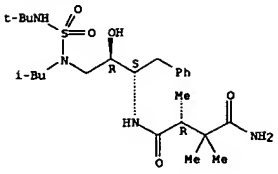
III

AB Title compds. [I; R1 = H, CH2-SO2-NH2, CH2-CO2Me, CO2Me, CONH2, CH2-CO-NHMe, CMe2-SH, etc.; R2 = alkyl, aryl, cycloalkyl, cycloalkylalkyl, NO2, cyano, CF3, OH, SH, alkoxy, etc.; R3 = alkyl, haloalkyl, alkenyl, alkynyl, hydroxyalkyl, alkoxyalkyl, cycloalkyl, etc.; R4, R5 = H, any group in the definition of R3; R6 = H, alkyl; R30,R31,R32 = H, alkyl, alkenyl, alkynyl, etc.; R33, R34 = H, any group in the definition of R3, or R33 and R34 together with X = cycloalkyl, aryl, heterocyclyl, heteroaryl provided that when X = O, R34 = nil; X = N, O, CR17; R17 = H, alkyl; x = 1, 2; t = 0, 1, 2; Y, Y1 = O, S, NR15; R15 = H, any group in the definition of R3], effective as retroviral protease inhibitors, and in particular as inhibitors of HIV protease, are prepared Thus, 4-benzyl-2(R),3,3-trimethylsuccinate was condensed with the [(tert-butylaminosulfonyl)amino]propylamine derivative II (preparation given) in DMF containing HOBt and 1-(3-dimethylaminopropyl)-3-ethylcarbodiimide hydrochloride to give the title compound III. III had an IC50 of 1.4 μM against retroviral protease in an in vitro study. The title compds. were also compared with AZT in a CEM cell assay.

IT 160765-56-0P 160765-57-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of, as retroviral protease inhibitor)
RN 160765-56-0 CAPLUS
CN Butanediamide, N4-[(1S,2R)-3-[[[(1,1-dimethylethyl)amino]sulfonyl](2-methylpropyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-2,2,3-trimethyl-, (3R)- (9CI) (CA INDEX NAME)

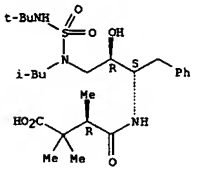
Absolute stereochemistry.

L4 ANSWER 19 OF 23 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



RN 160765-57-1 CAPLUS
CN 4-Thia-3,5,9-triazatridecan-13-oic acid, 7-hydroxy-2,2,11,12,12-pentamethyl-5-(2-methylpropyl)-10-oxo-8-(phenylmethyl)-, 4,4-dioxide, [7R-(7R*,8S*,11R*)]- (9CI) (CA INDEX NAME)

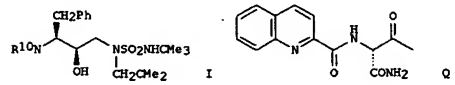
Absolute stereochemistry.



L4 ANSWER 20 OF 23 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1995:330514 CAPLUS
DOCUMENT NUMBER: 122:106521
TITLE: Preparation of N-sulfamidohydroxyalkyl amino acid amides as retroviral protease inhibitors
INVENTOR(S): Vazquez, Michael L.; Mueller, Richard A.; Talley, John J.; Getman, Daniel P.; Decrescenzo, Gary A.; Sun, Eric T.
PATENT ASSIGNEE(S): G.D. Searle and Co., USA; Monsanto Co.
SOURCE: PCT Int. Appl., 153 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9410134	A1	19940511	WO 1993-US10552	19931029
W: AT, AU, BB, BG, BR, BY, CA, CH, CZ, DE, DK, ES, FI, GB, HU, JP, KP, KR, KZ, LK, LU, LV, MG, MN, MW, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SK, UA, US, VN				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
CA 2142997	AA	19940511	CA 1993-2142997	19931029
AU 9455470	A1	19940524	AU 1994-55470	19931029
EP 666842	A1	19950816	EP 1994-900506	19931029
EP 666842	B1	19980624		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
EP 810208	A2	19971203	EP 1997-113206	19931029
EP 810208	A3	19981202		
EP 810208	B1	20020102		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE				
AT 167669	E	19980715	AT 1994-900506	19931029
ES 2118364	T3	19980916	ES 1994-900506	19931029
AT 211462	E	20020115	AT 1997-113206	19931029
PT 810208	T	20020628	PT 1997-113206	19931029
ES 2170305	T3	20020801	ES 1997-113206	19931029
US 6156768	A	20001205	US 1995-379545	19950202
US 6444678	B1	20020903	US 2000-633063	20000804
US 2003158236	A1	20030821	US 2002-178956	20020625
PRIORITY APPLN. INFO.:			US 1992-968730 A	19921030
			EP 1994-900506 A3	19931029
			WO 1993-US10552 W	19931029
			US 1995-379545 A3	19950202
			US 2000-633063 A1	20000804

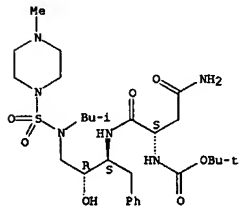
OTHER SOURCE(S): MARPAT 122:106521
GI



AB RR'N(CR7R8)tCHR1C(:Y)NR6CHR2CH(OH)CH2NR3SOxNR4R5 [R = H, (cyclo)alkyl, (hetero)aryl, alkyl(oxy)carbonyl, heterocyclyl(oxy)carbonyl, etc.; R' =

L4 ANSWER 20 OF 23 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
groups cited for R3, R''SO2; R'' = groups cited for R3; NRR' = heterocyclyl, heteroaryl; R1,R7,R8 = H, (halo)alkyl, amino acid side chain, CONH2, CO2Me, etc.; R1R7 = atoms to form a cycloalkyl group; R2 = (un)substituted (cyclo)alkyl, aryl(alkyl); R3 = (cyclo)alkyl, (hetero)aryl(alkyl), aminoalkyl, etc.; R4,R5 = H, groups cited for R3; NR4R5 = heterocyclyl, heteroaryl; R6 = H, alkyl; Y = O, S, NH, NR3; t = 0-2; x = 1 or 2] were prepd. Thus, N-benzyloxycarbonyl-3(S)-amino-1,2(S)-epoxy-4-phenylbutane (prepn. given) was condensed with Me2CHCH2NH2 and the product amidated by ClSO2NHCMe3 (prepn. given) to give, after deprotection, sulfamamide I (R10 = H) which was N-acylated by N-BOC-L-asparagine and the deprotected product N-acylated by quinoline-2-carboxylic acid to give I (R10 = quinolinoylasparaginyl group Q). The latter had IC50 of 2nM against HIV-1 infection of CEM cells in vitro.
IT **160677-10-1P 160677-11-2P 160677-13-4P 160677-14-5P 160677-15-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, in preparation of retroviral protease inhibitor)
RN 160677-10-1 CAPLUS
CN Carbamic acid, [3-amino-1-[[[2-hydroxy-3-[[(4-methyl-1-piperazinyl)sulfonyl](2-methylpropyl)amino]-1-(phenylmethyl)propyl]amino]carbonyl]-3-oxopropyl]-, 1,1-dimethylethyl ester, [1S-[1R*(R*),2S*]]- (9CI) (CA INDEX NAME)

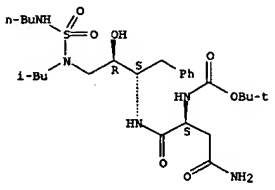
Absolute stereochemistry.



RN 160677-11-2 CAPLUS
CN 10-Thia-2,5,9,11-tetraazapentadecanoic acid, 3-(2-amino-2-oxoethyl)-7-hydroxy-9-(2-methylpropyl)-4-oxo-6-(phenylmethyl)-, 1,1-dimethylethyl ester, 10,10-dioxide, [3S-(3R*,6R*,7S*)]- (9CI) (CA INDEX NAME)

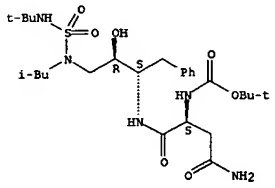
Absolute stereochemistry.

L4 ANSWER 20 OF 23 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



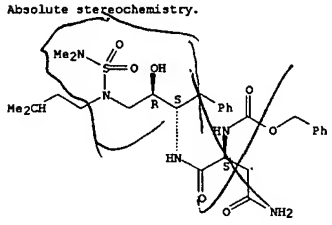
RN 160677-13-4 CAPLUS
CN 10-Thia-2,5,9,11-tetraazatridecanoic acid, 3-(2-amino-2-oxoethyl)-7-hydroxy-12,12-dimethyl-9-(2-methylpropyl)-4-oxo-6-(phenylmethyl)-, 1,1-dimethylethyl ester, 10,10-dioxide, [3S-(3R*,6R*,7S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 160677-14-5 CAPLUS
CN 3-Thia-2,4,8,11-tetraazadodecan-12-oic acid, 10-(2-amino-2-oxoethyl)-6-hydroxy-2-methyl-4-(3-methylbutyl)-9-oxo-7-(phenylmethyl)-, phenylmethyl ester, 3,3-dioxide, [6R-(6R*,7S*,10S*)]- (9CI) (CA INDEX NAME)

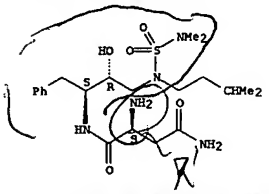
Absolute stereochemistry.



L4 ANSWER 20 OF 23 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 160677-15-6 CAPLUS
CN Butanediamide, 2-amino-N1-[3-[[(dimethylamino)sulfonyl](3-methylbutyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-, [1S-[1R*(R*),2S*]]- (9CI) (CA INDEX NAME)

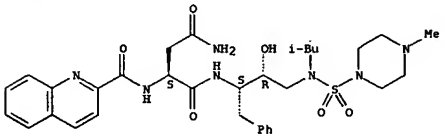
Absolute stereochemistry.



IT **160676-90-4P 160676-91-5P 160676-92-6P 160676-93-7P 160676-94-8P 160677-16-7P 160677-18-9P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of, as retroviral protease inhibitor)

RN 160676-90-4 CAPLUS
CN Butanediamide, N1-[3-[[(4-methyl-1-piperazinyl)sulfonyl](2-methylpropyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, [1S-[1R*(R*),2S*]]- (9CI) (CA INDEX NAME)

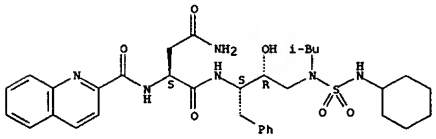
Absolute stereochemistry.



RN 160676-91-5 CAPLUS
CN Butanediamide, N1-[3-[[(butylamino)sulfonyl](2-methylpropyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, [1S-[1R*(R*),2S*]]- (9CI) (CA INDEX NAME)

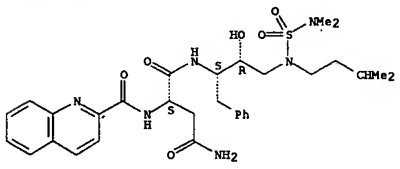
Absolute stereochemistry.

L4 ANSWER 20 OF 23 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



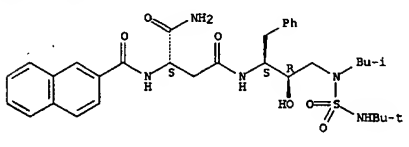
RN 160677-16-7 CAPLUS
CN Butanediamide, N1-[3-[[(dimethylamino)sulfonyl](3-methylbutyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, [1S-[1R*(R*),2S*]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

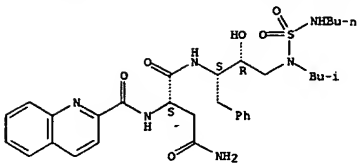


RN 160677-18-9 CAPLUS
CN Butanediamide, N4-[(1S,2R)-3-[[[(1,1-dimethylethyl)amino]sulfonyl](2-methylpropyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-naphthalenylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

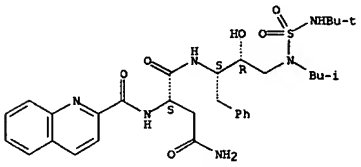


L4 ANSWER 20 OF 23 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



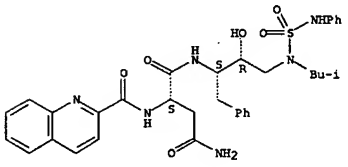
RN 160676-92-6 CAPLUS
CN Butanediamide, N1-[3-[[[(1,1-dimethylethyl)amino]sulfonyl](2-methylpropyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, [1S-[1R*(R*),2S*]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 160676-93-7 CAPLUS
CN Butanediamide, N1-[2-hydroxy-3-[(2-methylpropyl)[(phenylamino)sulfonyl]amino]-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, [1S-[1R*(R*),2S*]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 160676-94-8 CAPLUS
CN Butanediamide, N1-[3-[[(cyclohexylamino)sulfonyl](2-methylpropyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, [1S-[1R*(R*),2S*]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 21 OF 23 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1995:293723 CAPLUS
DOCUMENT NUMBER: 122:81141
TITLE: Preparation of heterocyclylarylsulfonamide inhibitors of HIV-aspartyl protease
INVENTOR(S): Tung, Roger D.; Murcko, Mark A.; Bhisetti, Govinda Rao
PATENT ASSIGNEE(S): Vertex Pharmaceuticals Inc., USA
SOURCE: PCT Int. Appl., 291 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 5
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9405639	A1	19940317	WO 1993-US8458	19930907
W: AT, AU, BB, BG, BR, BY, CA, CH, CZ, DE, DK, ES, FI, GB, HU, JP, KP, KR, KZ, LK, LU, LV, MG, MN, MW, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SK, UA, US, UZ, VN				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
LT 3302	B	19950626	LT 1993-917	19930901
IL 106927	A1	20010111	IL 1993-106927	19930906
EP 659181	A1	19950628	EP 1993-921428	19930907
EP 659181	B1	19990407		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
JP 08501299	T2	19960213	JP 1994-507525	19930907
HU 71892	A2	19960228	HU 1995-685	19930907
AU 691160	B2	19980514	AU 1993-48520	19930907
AU 9348520	A1	19940329		
EP 885887	A2	19981223	EP 1998-113921	19930907
EP 885887	A3	19990203		
EP 885887	B1	20030528		
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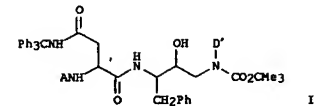
AT 178598	E	19990415	AT 1993-921428	19930907
ES 2131589	T3	19990801	ES 1993-921428	19930907
RU 2135496	C1	19990827	RU 1995-109928	19930907
SK 281360	B6	20010212	SK 1995-293	19930907
CZ 289475	B6	20020116	CZ 1995-587	19930907
CA 2143208	C	20030107	CA 1993-2143208	19930907
AT 241602	E	20030615	AT 1998-113921	19930907
PL 185635	B1	20030630	PL 1993-307858	19930907
RO 118747	B1	20031030	RO 1995-479	19930907
PT 885887	T	20031031	PT 1998-113921	19930907
ES 2200243	T3	20040301	ES 1998-113921	19930907
CN 1087347	A	19940601	CN 1993-117370	19930908
CN 1061339	B	20010131		
ZA 9308470	A	19940620	ZA 1993-8470	19931112
US 5585397	A	19961217	US 1993-142327	19931124
FI 9501059	A	19950418	FI 1995-1059	19950307
NO 9500876	A	19950508	NO 1995-876	19950307
NO 303444	B1	19980713		
HK 1012631	A1	20000623	HK 1998-113971	19981217
HK 1023561	A1	20040716	HK 2000-100689	19981217

PRIORITY APPLN. INFO.: US 1992-941982 A2 19920908
EP 1993-921428 A3 19930907
WO 1993-US8458 W 19930907

OTHER SOURCE(S): MARPAT 122:81141
GI



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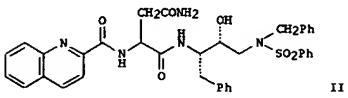

II

AB Title compds. A(B)xNHCH(D)CH(OH)CH2N(D')SO2E (A = H, Het, R1-Het, (substituted)R1-C1-6 alkyl, (substituted) R1-C2-6 alkenyl wherein R1 = CO, SO2, COCO, O2C, etc., Het = C5-7 cycloalkyl, C5-7 cycloalkenyl, C6-10 aryl, (substituted) 5-7-membered heterocyclyl; R2 = H, (Ar)-C1-3 alkyl; B = NR2CR3CO, null wherein R3 = H, (substituted)Het or C1-6 alkyl or C2-6 alkenyl or C3-6 cycloalkyl or C5-6 cycloalkenyl; x = 0,1; D, D' = Ar, (substituted) C1-4 alkyl wherein Ar = Ph, (substituted) 3-6-membered carbocyclyl or 5-6-membered heterocyclyl; E = Het-O, Het-Het, (substituted) C1-6 alkyl or C2-6 alkenyl, C3-6 carbocyclyl) useful also against viral infection of HIV-2, HIV-2, or HTLV, are prepared 4,3-(AcNH)FC6H3SO2Cl and syn-I (A = quinolin-2-ylcarbonyl, D' = Me2CHCH2) (preparation given) in CH2Cl2 was treated with F3CCO2H followed by NaHCO3 and 4-FC6H4SO2Cl to give the title compound II which inhibited HIV-1 protease with IC50 of <0.1 nM.

IT **160230-05-7P 160230-06-8P 160230-07-9P**
160230-08-0P 160230-09-1P 160230-10-4P
160230-11-5P 160230-12-6P 160230-13-7P
160230-14-8P 160230-15-9P 160230-16-0P
160230-17-1P 160230-18-2P 160230-19-3P
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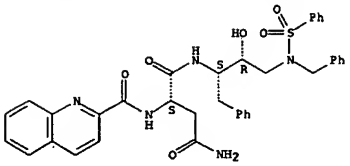
160230-50-2P 160231-93-6P 160231-96-9P
160333-42-6P 160333-43-7P 160333-44-8P
160333-45-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of as HIV-1 protease inhibitor)

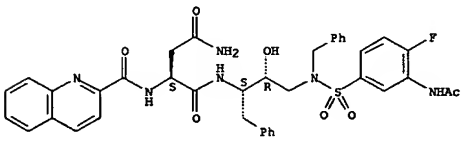
RN 160230-05-7 CAPLUS
CN Butanediamide, N1-[(1S,2R)-2-hydroxy-1-(phenylmethyl)-3-[(phenylmethyl)(phenylsulfonyl)amino]propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



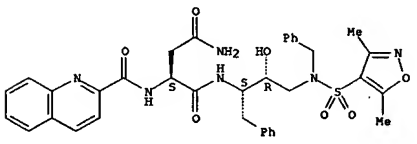
RN 160230-06-8 CAPLUS
CN Butanediamide, N1-[(1S,2R)-3-[[[3-(acetylamino)-4-fluorophenyl]sulfonyl](phenylmethyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



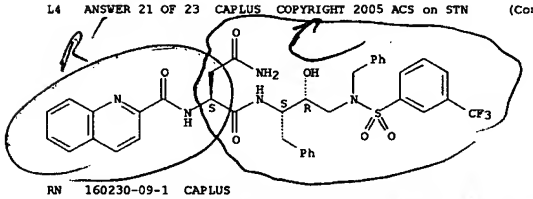
RN 160230-07-9 CAPLUS
CN Butanediamide, N1-[(1S,2R)-3-[[(3,5-dimethyl-4-isoxazolyl)sulfonyl](phenylmethyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



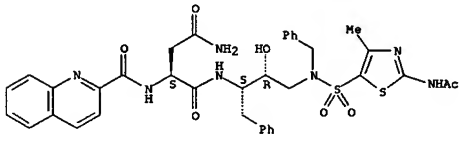
RN 160230-08-0 CAPLUS
CN Butanediamide, N1-[(1S,2R)-2-hydroxy-1-(phenylmethyl)-3-[(phenylmethyl)[[3-(trifluoromethyl)phenyl]sulfonyl]amino]propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



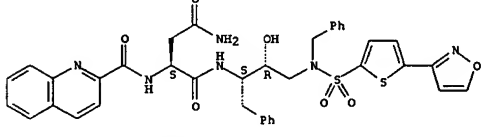
RN 160230-09-1 CAPLUS
CN Butanediamide, N1-[(1S,2R)-3-[[[2-(acetylamino)-4-methyl-5-thiazolyl]sulfonyl](phenylmethyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



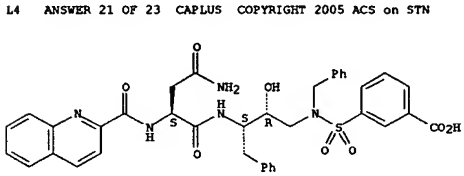
RN 160230-10-4 CAPLUS
CN Butanediamide, N1-[(1S,2R)-2-hydroxy-3-[[[5-(3-isoxazolyl)-2-thienyl]sulfonyl](phenylmethyl)amino]-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



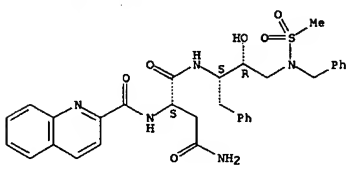
RN 160230-11-5 CAPLUS
CN Benzoic acid, 3-[[[(2R,3S)-3-[[(2S)-4-amino-1,4-dioxo-2-[(2-quinolinylcarbonyl)amino]butyl]amino]-2-hydroxy-4-phenylbutyl](phenylmethyl)amino]sulfonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



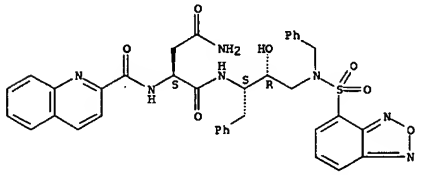
RN 160230-12-6 CAPLUS
CN Butanediamide, N1-[(1S,2R)-2-hydroxy-3-[(methylsulfonyl)(phenylmethyl)amino]-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



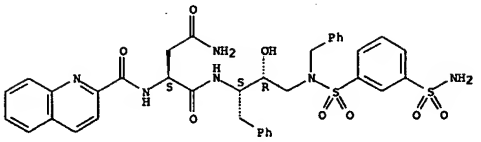
RN 160230-13-7 CAPLUS
CN Butanediamide, N1-[(1S,2R)-3-[(2,1,3-benzoxadiazol-4-ylsulfonyl)(phenylmethyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



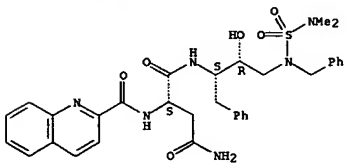
RN 160230-14-8 CAPLUS
CN Butanediamide, N1-[(1S,2R)-3-[[[3-(aminosulfonyl)phenyl]sulfonyl](phenylmethyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



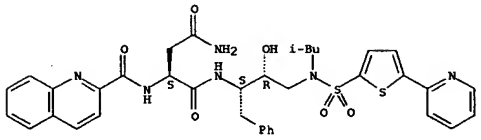
RN 160230-15-9 CAPLUS
CN Butanediamide, N1-[(1S,2R)-3-[[(dimethylamino)sulfonyl](phenylmethyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



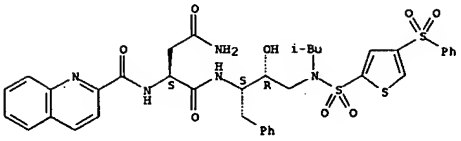
RN 160230-16-0 CAPLUS
CN Butanediamide, N1-[(1S,2R)-2-hydroxy-3-[(2-methylpropyl)[[5-(2-pyridinyl)-2-thienyl]sulfonyl]amino]-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



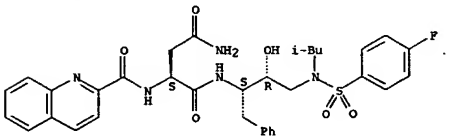
RN 160230-17-1 CAPLUS
CN Butanediamide, N1-[(1S,2R)-2-hydroxy-3-[(2-methylpropyl)[[4-(phenylsulfonyl)-2-thienyl]sulfonyl]amino]-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



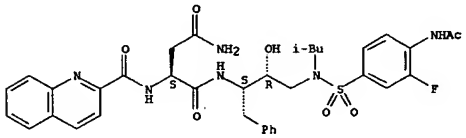
RN 160230-18-2 CAPLUS
CN Butanediamide, N1-[(1S,2R)-3-[[(4-fluorophenyl)sulfonyl](2-methylpropyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



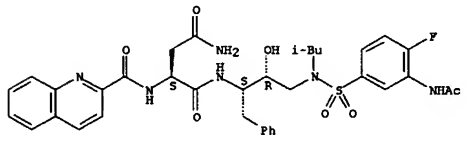
RN 160230-19-3 CAPLUS
CN Butanediamide, N1-[(1S,2R)-3-[[[4-(acetylamino)-3-fluorophenyl]sulfonyl](2-methylpropyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



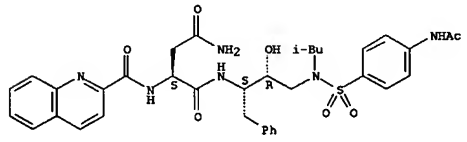
RN 160230-20-6 CAPLUS
CN Butanediamide, N1-[(1S,2R)-3-[[[3-(acetylamino)-4-fluorophenyl]sulfonyl](2-methylpropyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



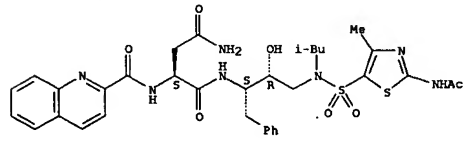
RN 160230-21-7 CAPLUS
CN Butanediamide, N1-[(1S,2R)-3-[[[4-(acetylamino)phenyl]sulfonyl](2-methylpropyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



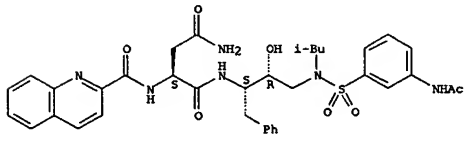
RN 160230-22-8 CAPLUS
CN Butanediamide, N1-[(1S,2R)-3-[[[2-(acetylamino)-4-methyl-5-thiazolyl]sulfonyl](2-methylpropyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 160230-23-9 CAPLUS
CN Butanediamide, N1-[(1S,2R)-3-[[[3-(acetylamino)phenyl]sulfonyl](2-methylpropyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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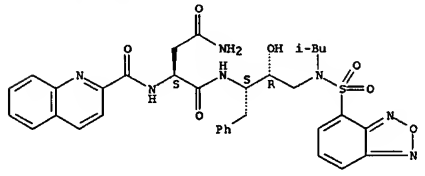
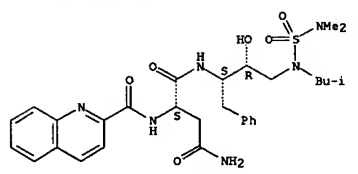
CN Butanediamide, N1-[(1S,2R)-3-[(2,1,3-benzoxadiazol-4-ylsulfonyl)(2-methylpropyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



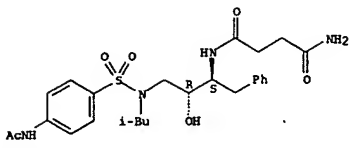
RN 160230-25-1 CAPLUS
CN Butanediamide, N1-[(1S,2R)-3-[[(dimethylamino)sulfonyl](2-methylpropyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



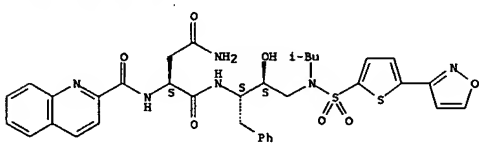
RN 160230-50-2 CAPLUS
CN Butanediamide, N-[(1S,2R)-3-[[[4-(acetylamino)phenyl]sulfonyl](2-methylpropyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



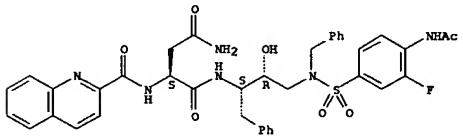
RN 160231-93-6 CAPLUS
CN Butanediamide, N1-{(1S,2S)-2-hydroxy-3-[[[5-(3-isoxazolyl)-2-thienyl]sulfonyl](2-methylpropyl)amino]-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 160231-96-9 CAPLUS
CN Butanediamide, N1-[(1S,2R)-3-[[[4-(acetylamino)-3-fluorophenyl]sulfonyl](phenylmethyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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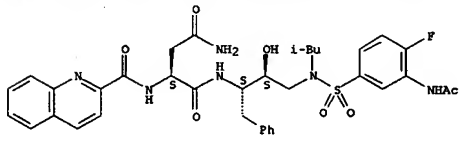
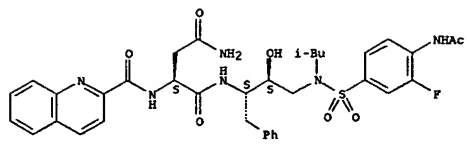
Absolute stereochemistry.





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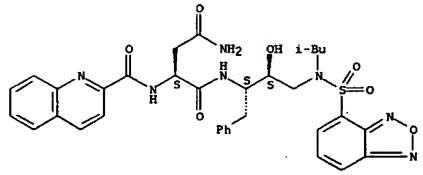
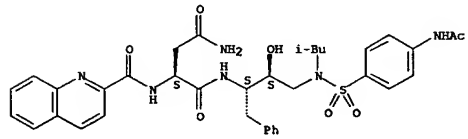
CN Butanediamide, N1-[(1S,2S)-3-[(2,1,3-benzoxadiazol-4-ylsulfonyl)(2-methylpropyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 160333-44-8 CAPLUS
CN Butanediamide, N1-[(1S,2S)-3-[[[4-(acetylamino)phenyl]sulfonyl](2-methylpropyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 160333-45-9 CAPLUS
CN Butanediamide, N1-[(1S,2S)-3-[[[3-(acetylamino)-4-fluorophenyl]sulfonyl](2-methylpropyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ACCESSION NUMBER: 1994:701324 CAPLUS
DOCUMENT NUMBER: 121:301324
TITLE: Preparation of hydroxyethylamino sulfonamides useful as retroviral protease inhibitors
INVENTOR(S): Vazquez, Michael L.; Mueller, Richard A.; Talley, John J.; Getman, Daniel; Decrescenzo, Gary A.; Freskos, John N.
PATENT ASSIGNEE(S): G.D. Searle and Co., USA; Monsanto Co.
SOURCE: PCT Int. Appl., 198 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 6
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9404492	A1	19940303	WO 1993-US7814	19930824
W: AT, AU, BB, BG, BR, BY, CA, CH, CZ, DE, DK, ES, FI, GB, HU, JP, KP, KR, KZ, LK, LU, MG, MN, MW, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SK, UA, US, VN				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
EP 656887	A1	19950614	EP 1993-923714	19930824
EP 656887	B1	19981028		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
JP 08501288	T2	19960213	JP 1994-506530	19930824
JP 3657002	B2	20050608		
AU 680635	B2	19970807	AU 1994-53474	19930824
AU 9453474	A1	19940315		
EP 810209	A2	19971203	EP 1997-113434	19930824
EP 810209	A3	19981202		
EP 810209	B1	20020605		
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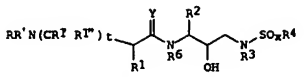
AT 172717	E	19981115	AT 1993-923714	19930824
ES 2123065	T3	19990101	ES 1993-923714	19930824
RU 2173680	C2	20010920	RU 1995-106624	19930824
AT 218541	E	20020615	AT 1997-113434	19930824
PT 810209	T	20020930	PT 1997-113434	19930824
ES 2177868	T3	20021216	ES 1997-113434	19930824
US 6060476	A	20000509	US 1994-204827	19940302
US 5968942	A	19991019	US 1994-294468	19940823
NO 9500533	A	19950213	NO 1995-533	19950213
FI 9500650	A	19950214	FI 1995-650	19950214
FI 112471	B1	20031215		
US 6455581	B1	20020924	US 1995-451090	19950525
US 6046190	A	20000404	US 1996-586866	19960124
NO 9803099	A	19950213	NO 1998-3099	19980703
NO 307047	B1	20000131		
US 6248775	B1	20010619	US 1999-288080	19990408
US 6500832	B1	20021231	US 2000-525161	20000314
US 2002052399	A1	20020502	US 2001-798255	20010305
US 6417387	B2	20020709		
FI 2001002317	A	20011127	FI 2001-2317	20011127
US 2003191319	A1	20031009	US 2002-157019	20020530
US 6646010	B2	20031111		
US 2004044047	A1	20040304	US 2002-199481	20020722
US 6846954	B2	20050125		
US 6924286	B1	20050802	US 2003-633376	20030804
US 2004229922	A1	20041118	US 2004-812343	20040330

PRIORITY APPLN. INFO.:
US 1992-934984 A2 19920825
EP 1993-923714 A3 19930824
US 1993-110911 A2 19930824
WO 1993-US7814 W 19930824
US 1994-204827 A2 19940302
US 1994-204872 B2 19940302
US 1994-294468 A1 19940823
WO 1994-US9139 W 19940823
US 1995-451090 A3 19950525
US 1999-288080 A1 19990408
US 2001-798255 A1 20010305
US 2002-157019 A1 20020530
US 2002-199481 A3 20020722

OTHER SOURCE(S): MARPAT 121:301324

GI



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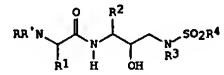

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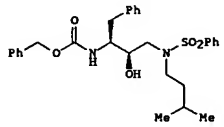


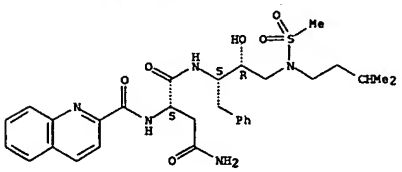
III

AB Title compds. [I and II; R = H, alkoxycarbonyl, aralkoxycarbonyl, alkylcarbonyl, cycloalkylcarbonyl, heterocyclylcarbonyl, heteroaryloxyalkyl, hydroxyalkyl, aryl, alkyl, alkenyl, alkynyl, substituted aminocarbonyl, etc.; R' = H, R3, R''SO2; RR'N = heterocyclyl, heteroaryl; R1 = H, CH2SO2NH2, CH2CO2Me, CO2Me, CONH2, CMe2SH, alkyl, haloalkyl, alkenyl, alkynyl, cycloalkyl, amino acid side chains, etc.; R1', R1'' = H, R1; 1 of R1', R1'' together with R1 form a cycloalkyl radical; R2 = (substituted) alkyl, aryl, cycloalkyl, cycloalkylalkyl, aralkyl; R3 = H, alkyl, haloalkyl, alkenyl, alkynyl, hydroxyalkyl, alkoxyalkyl, cycloalkyl, heterocycloalkyl, heteroaryl, aryl, aralkyl, heteroaralkyl, (substituted) aminoalkyl, etc.; R4 = R3, except H; R6 = H, alkyl; x = 0-2; t = 0, 1; Y = O, S, imino], were prepared Thus, title compound (III, solution phase preparation given) inhibited HIV protease with IC50 = 16 nM.

IT **159005-89-7P 159005-90-0P 159005-91-1P 159005-92-2P 159005-95-5P 159006-21-0P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. of, as HIV protease inhibitor)

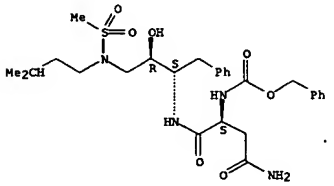
RN 159005-89-7 CAPLUS
CN Butanediamide, N1-[(1S,2R)-2-hydroxy-3-[(3-methylbutyl)(methylsulfonyl)amino]-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



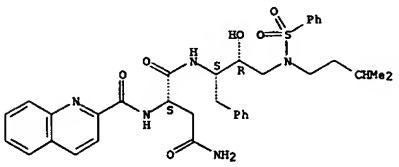
RN 159005-90-0 CAPLUS
CN 2-Thia-3,7,10-triazaundecan-11-oic acid, 9-(2-amino-2-oxoethyl)-5-hydroxy-3-(3-methylbutyl)-8-oxo-6-(phenylmethyl)-, phenylmethyl ester, 2,2-dioxide, (5R,6S,9S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



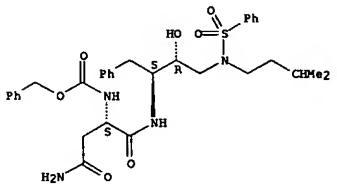
RN 159005-91-1 CAPLUS
CN Butanediamide, N1-[(1S,2R)-2-hydroxy-3-[(3-methylbutyl)(phenylsulfonyl)amino]-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



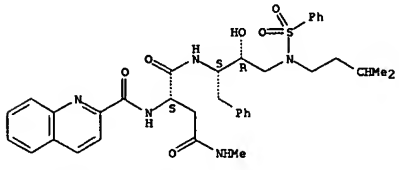
RN 159005-92-2 CAPLUS
CN Carbamic acid, [(1S)-3-amino-1-[[[(1S,2R)-2-hydroxy-3-[(3-methylbutyl)(phenylsulfonyl)amino]-1-(phenylmethyl)propyl]amino]carbonyl]-3-oxopropyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



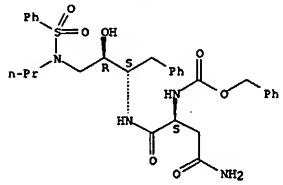
RN 159005-95-5 CAPLUS
CN Butanediamide, N1-[(1S,2R)-2-hydroxy-3-[(3-methylbutyl)(phenylsulfonyl)amino]-1-(phenylmethyl)propyl]-N4-methyl-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 159006-21-0 CAPLUS
CN Carbamic acid, [(1S)-3-amino-1-[[[(1S,2R)-2-hydroxy-1-(phenylmethyl)-3-[(phenylsulfonyl)propylamino]propyl]amino]carbonyl]-3-oxopropyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

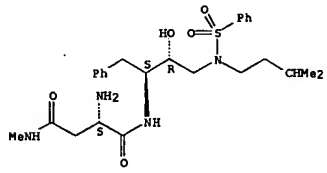
Absolute stereochemistry.



IT **159006-49-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as HIV protease inhibitor intermediate)

RN 159006-49-2 CAPLUS
CN Butanediamide, 2-amino-N1-[2-hydroxy-3-[(3-methylbutyl)(phenylsulfonyl)amino]-1-(phenylmethyl)propyl]-N4-methyl-, monohydrochloride, [1S-[1R*(R*),2S*]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

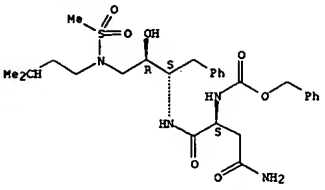


● HCl

IT **159005-90-0P 159005-92-2P 159006-05-0P 159006-06-1P 159006-22-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as intermediate for HIV protease inhibitor)

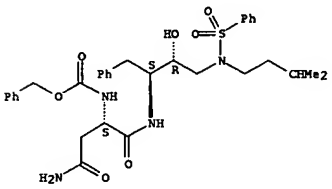
RN 159005-90-0 CAPLUS
CN 2-Thia-3,7,10-triazaundecan-11-oic acid, 9-(2-amino-2-oxoethyl)-5-hydroxy-3-(3-methylbutyl)-8-oxo-6-(phenylmethyl)-, phenylmethyl ester, 2,2-dioxide, (5R,6S,9S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



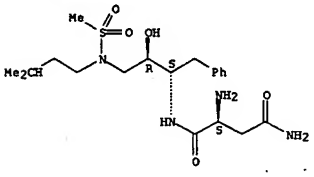
RN 159005-92-2 CAPLUS
CN Carbamic acid, [(1S)-3-amino-1-[[[(1S,2R)-2-hydroxy-3-[(3-methylbutyl)(phenylsulfonyl)amino]-1-(phenylmethyl)propyl]amino]carbonyl]-3-oxopropyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 159006-05-0 CAPLUS
CN Butanediamide, 2-amino-N1-[(1S,2R)-2-hydroxy-3-[(3-methylbutyl)(methylsulfonyl)amino]-1-(phenylmethyl)propyl]-, (2S)- (9CI) (CA INDEX NAME)

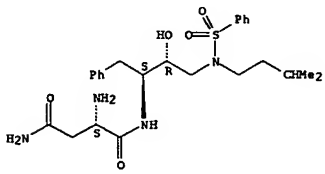
Absolute stereochemistry.



RN 159006-06-1 CAPLUS

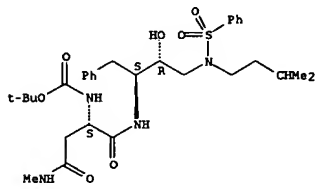
CN Butanediamide, 2-amino-N1-[(1S,2R)-2-hydroxy-3-[(3-methylbutyl)(phenylsulfonyl)amino]-1-(phenylmethyl)propyl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 159006-22-1 CAPLUS
CN Carbamic acid, [(1S)-1-[[[(1S,2R)-2-hydroxy-3-[(3-methylbutyl)(phenylsulfonyl)amino]-1-(phenylmethyl)propyl]amino]carbonyl]-3-(methylamino)-3-oxopropyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



ACCESSION NUMBER: 1994:579258 CAPLUS
DOCUMENT NUMBER: 121:179258
TITLE: N-(alkanoylamino-2-hydroxypropyl)sulfonamides useful as HIV protease inhibitors
INVENTOR(S): Vazquez, Michael L.; Mueller, Richard A.; Talley, John J.; Getman, Daniel; Decrescenzo, Gary A.; Freskos, John N.
PATENT ASSIGNEE(S): G.D. Searle and Co., USA; Monsanto Co.
SOURCE: PCT Int. Appl., 103 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9404491	A1	19940303	WO 1993-US7815	19930825
W: AT, AU, BB, BG, BR, BY, CA, CH, CZ, DE, DK, ES, FI, GB, HU, JP, KP, KR, KZ, LK, LU, MG, MN, MW, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SK, UA, US, VN				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
EP 656886	A1	19950614	EP 1993-920213	19930824
EP 656886	B1	19970625		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
JP 08500824	T2	19960130	JP 1993-506531	19930824
AT 154800	E	19970715	AT 1993-920213	19930824
ES 2103488	T3	19970916	ES 1993-920213	19930824
AU 674702	B2	19970109	AU 1993-50819	19930825
AU 9350819	A1	19940315		
RU 2130016	C1	19990510	RU 1995-106823	19930825
NO 9500670	A	19950222	NO 1995-670	19950222
FI 9500841	A	19950223	FI 1995-841	19950223
PRIORITY APPLN. INFO.:			US 1992-935490	A2 19920825
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OTHER SOURCE(S): MARPAT 121:179258
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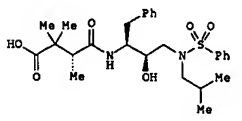


I

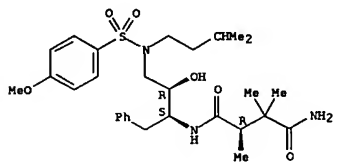
AB The title compds. R33(R34)X1C(:Y1)(CH2)tC(R31)(R32)C(R30)(R1)C(:Y)N(R6)C(R2)HC(OH)HCH2N(R3)S(O)xR4 [R1 = H, CH2SO2NH2, CO2Me, CONHMe, CONMe2, etc.; R2 = alkyl, aryl, cycloalkyl, (un)substituted cycloalkylalkyl and arylalkyl; R3 = H, alkyl, haloalkyl, alkenyl, alkynyl, hydroxyalkyl, alkoxyalkyl, cycloalkyl, etc.; R4 = alkyl, haloalkyl alkenyl, alkynyl, hydroxyalkyl, alkoxyalkyl, cycloalkyl etc.; R6 = H, alkyl; R30-R32 = R1; R1R30R31 = cycloalkyl; R1R30R32C = cycloalkyl; R33, R34 = H, R3; R33R34X1

= cycloalkyl, aryl, heterocyclyl, etc.; X1 = O, N, CR17; R17 = H, alkyl; Y, Y1 = O, S, NR15; R15 = H, R3; t = 0, 1; x = 0-2], useful as HIV protease inhibitors for the treatment of AIDS, are prepd. Thus, sulfonamide I was prepd. and demonstrated IC50 against HIV protease of 1 nmol.

IT **157446-05-4 157446-06-5 157446-07-6**
157446-08-7 157446-09-8 157474-44-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(HIV protease inhibitor)

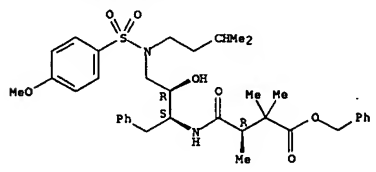
RN 157446-05-4 CAPLUS
CN Butanediamide, N4-[(1S,2R)-2-hydroxy-3-[[(4-methoxyphenyl)sulfonyl](3-methylbutyl)amino]-1-(phenylmethyl)propyl]-2,2,3-trimethyl-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



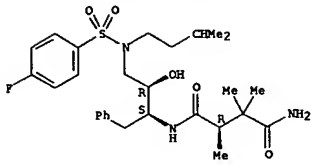
RN 157446-06-5 CAPLUS
CN Butanoic acid, 4-[[2-hydroxy-3-[[(4-methoxyphenyl)sulfonyl](3-methylbutyl)amino]-1-(phenylmethyl)propyl]amino]-2,2,3-trimethyl-4-oxo-, phenylmethyl ester, [1S-[1R*(S*),2S*]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



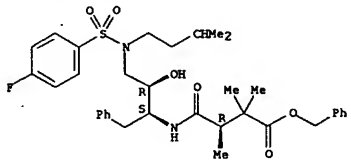
RN 157446-07-6 CAPLUS
CN Butanediamide, N4-[(1S,2R)-3-[[(4-fluorophenyl)sulfonyl](3-methylbutyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-2,2,3-trimethyl-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



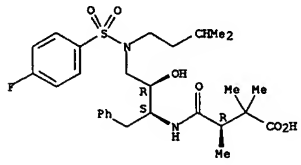
RN 157446-08-7 CAPLUS
CN Butanoic acid, 4-[[3-[[(4-fluorophenyl)sulfonyl](3-methylbutyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]amino]-2,2,3-trimethyl-4-oxo-, phenylmethyl ester, [1S-[1R*(S*),2S*]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



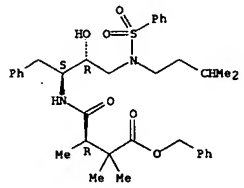
RN 157446-09-8 CAPLUS
CN Butanoic acid, 4-[[3-[[(4-fluorophenyl)sulfonyl](3-methylbutyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]amino]-2,2,3-trimethyl-4-oxo-, [1S-[1R*(S*),2S*]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



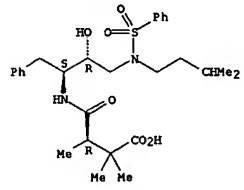
RN 157474-44-7 CAPLUS
CN Butanoic acid, 4-[[2-hydroxy-3-[[(4-methoxyphenyl)sulfonyl](3-methylbutyl)amino]-1-(phenylmethyl)propyl]amino]-2,2,3-trimethyl-4-oxo-, [1S-[1R*(S*),2S*]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



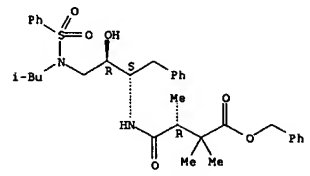
RN 157445-98-2 CAPLUS
CN Butanoic acid, 4-[[(1S,2R)-2-hydroxy-3-[(3-methylbutyl)(phenylsulfonyl)amino]-1-(phenylmethyl)propyl]amino]-2,2,3-trimethyl-4-oxo-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

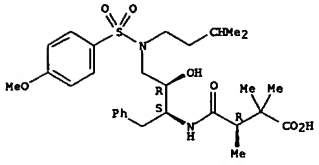


RN 157445-99-3 CAPLUS
CN Butanoic acid, 4-[[2-hydroxy-3-[(2-methylpropyl)(phenylsulfonyl)amino]-1-(phenylmethyl)propyl]amino]-2,2,3-trimethyl-4-oxo-, phenylmethyl ester, [1S-[1R*(S*),2S*]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

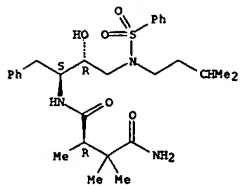


RN 157446-00-9 CAPLUS



IT 157445-96-0P 157445-97-1P 157445-98-2P
157445-99-3P 157446-00-9P 157446-02-1P
157446-03-2P 157446-04-3P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as HIV protease inhibitor)
RN 157445-96-0 CAPLUS
CN Butanediamide, N4-[(1S,2R)-2-hydroxy-3-[(3-methylbutyl)(phenylsulfonyl)amino]-1-(phenylmethyl)propyl]-2,2,3-trimethyl-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

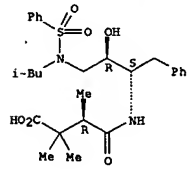


RN 157445-97-1 CAPLUS
CN Butanoic acid, 4-[[2-hydroxy-3-[(3-methylbutyl)(phenylsulfonyl)amino]-1-(phenylmethyl)propyl]amino]-2,2,3-trimethyl-4-oxo-, phenylmethyl ester, [1S-[1R*(S*),2S*]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

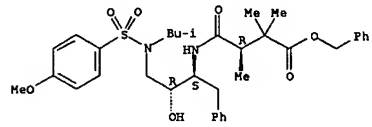
CN Butanoic acid, 4-[[2-hydroxy-3-[(2-methylpropyl)(phenylsulfonyl)amino]-1-(phenylmethyl)propyl]amino]-2,2,3-trimethyl-4-oxo-, [1S-[1R*(S*),2S*]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



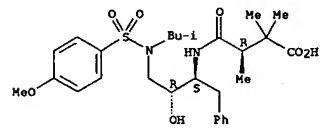
RN 157446-02-1 CAPLUS
CN Butanoic acid, 4-[[2-hydroxy-3-[[(4-methoxyphenyl)sulfonyl](2-methylpropyl)amino]-1-(phenylmethyl)propyl]amino]-2,2,3-trimethyl-4-oxo-, phenylmethyl ester, [1S-[1R*(S*),2S*]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 157446-03-2 CAPLUS
CN Butanoic acid, 4-[[2-hydroxy-3-[[(4-methoxyphenyl)sulfonyl](2-methylpropyl)amino]-1-(phenylmethyl)propyl]amino]-2,2,3-trimethyl-4-oxo-, [1S-[1R*(S*),2S*]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 157446-04-3 CAPLUS
CN Butanediamide, N4-[(1S,2R)-2-hydroxy-3-[[(4-methoxyphenyl)sulfonyl](2-methylpropyl)amino]-1-(phenylmethyl)propyl]-2,2,3-trimethyl-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.